



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:47 PM UTC

PDB ID : 8UGH / pdb_00008ugh
EMDB ID : EMD-42225
Title : In-situ structure of typeA supercomplex with lipids in respiratory chain (composite)
Authors : Zheng, W.; Zhang, K.; Zhu, J.
Deposited on : 2023-10-05
Resolution : 2.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

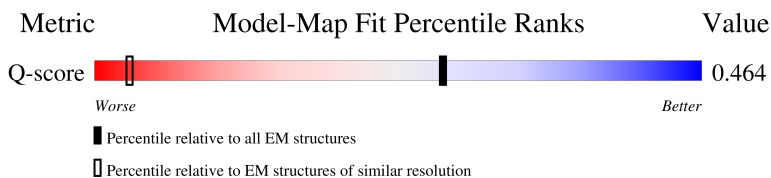
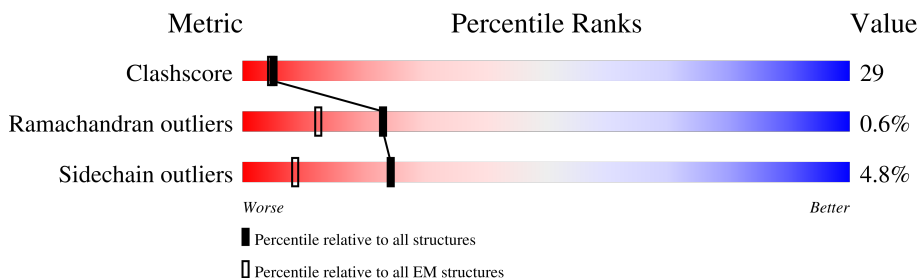
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	
2	1B	258	
3	1C	264	
4	1D	466	

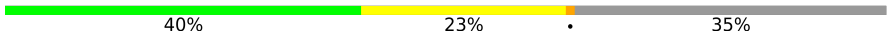
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	

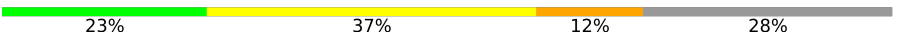
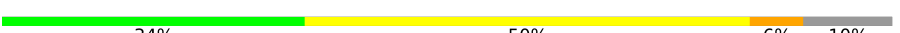
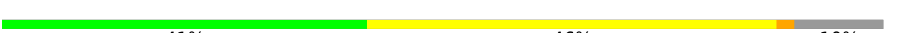
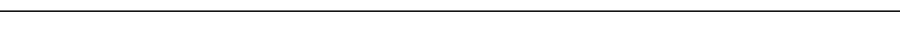
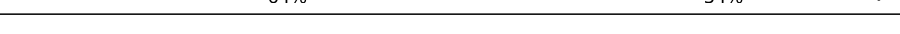
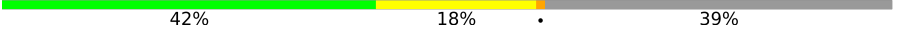
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Mol	Chain	Length	Quality of chain
29	1d	122	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	113	
44	1s	471	
45	3A	480	
45	3N	480	
46	3B	453	
46	3O	453	
47	3C	379	
47	3P	379	
48	3D	326	
48	3Q	326	
49	3E	274	

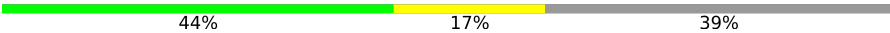
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Mol	Chain	Length	Quality of chain
49	3I	274	
49	3R	274	
49	3V	274	
50	3F	111	
50	3S	111	
51	3G	82	
51	3T	82	
52	3H	91	
52	3U	91	
53	3J	64	
53	3W	64	
54	3X	56	
54	3Y	56	
55	4A	514	
56	4B	229	
57	4C	261	
58	4D	169	
59	4E	152	
60	4F	129	
61	4G	97	
62	4H	86	
63	4I	75	
64	4J	80	
65	4K	80	
66	4L	63	

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Mol	Chain	Length	Quality of chain
67	4M	70	
68	4N	82	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	FME	4A	1	-	-	X	-
69	3PE	1B	204	-	-	X	-
69	3PE	1B	205	-	-	X	-
69	3PE	1J	201	-	-	X	-
69	3PE	1L	703	-	-	X	-
69	3PE	1L	709	-	-	X	-
69	3PE	1N	401	-	-	X	-
69	3PE	1Y	201	-	-	X	-
69	3PE	1Y	208	-	-	X	-
69	3PE	1Y	209	-	-	X	-
69	3PE	1Y	213	-	-	X	-
69	3PE	1Y	214	-	-	X	-
69	3PE	1Y	215	-	-	X	-
69	3PE	1b	101	-	-	X	-
69	3PE	1d	201	-	-	X	-
69	3PE	1d	203	-	-	X	-
69	3PE	1d	206	-	-	X	-
69	3PE	1f	104	-	-	X	-
69	3PE	1g	202	-	-	X	-
69	3PE	1k	101	-	-	X	-
69	3PE	1m	202	-	-	X	-
69	3PE	1m	203	-	-	X	-
69	3PE	1m	205	-	-	X	-
69	3PE	1o	201	-	-	X	-
69	3PE	3A	502	-	-	X	-
69	3PE	3A	503	-	-	X	-
69	3PE	3C	507	-	-	X	-
69	3PE	3C	508	-	-	X	-
69	3PE	3C	509	-	-	X	-
69	3PE	3C	511	-	-	X	-
69	3PE	3C	512	-	-	X	-
69	3PE	3C	513	-	-	X	-
69	3PE	3C	515	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
69	3PE	3C	516	-	-	X	-
69	3PE	3G	109	-	-	X	-
69	3PE	3N	501	-	-	X	-
69	3PE	3N	503	-	-	X	-
69	3PE	3P	503	-	-	X	-
69	3PE	3P	507	-	-	X	-
69	3PE	3P	508	-	-	X	-
69	3PE	3P	511	-	-	X	-
69	3PE	3P	514	-	-	X	-
69	3PE	3P	517	-	-	X	-
69	3PE	3P	518	-	-	X	-
69	3PE	3P	519	-	-	X	-
69	3PE	3P	520	-	-	X	-
69	3PE	3R	305	-	-	X	-
69	3PE	3S	201	-	-	X	-
69	3PE	3T	103	-	-	X	-
69	3PE	3W	101	-	-	X	-
69	3PE	3W	102	-	-	X	-
69	3PE	3W	103	-	-	X	-
69	3PE	3X	101	-	-	X	-
69	3PE	3X	105	-	-	X	-
69	3PE	3X	107	-	-	X	-
69	3PE	3X	108	-	-	X	-
69	3PE	3Y	102	-	-	X	-
69	3PE	3Y	105	-	-	X	-
69	3PE	3Y	107	-	-	X	-
69	3PE	4G	104	-	-	X	-
70	PC1	1A	202	-	-	X	-
70	PC1	1B	202	-	-	X	-
70	PC1	1B	203	-	-	X	-
70	PC1	1H	403	-	-	X	-
70	PC1	1Y	206	-	-	X	-
70	PC1	1Y	207	-	-	X	-
70	PC1	1d	204	-	-	X	-
70	PC1	3T	102	-	-	X	-
71	SF4	1F	502	-	-	X	-
71	SF4	1G	802	-	-	X	-
71	SF4	1I	202	-	-	X	-
72	FES	1E	301	-	-	X	-
72	FES	1G	803	-	-	X	-
72	FES	3E	301	-	-	X	-
72	FES	3R	301	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
75	CDL	1L	704	-	-	X	-
75	CDL	1N	402	-	-	X	-
75	CDL	1Y	217	-	-	X	-
75	CDL	1d	202	-	-	X	-
75	CDL	1d	205	-	-	X	-
75	CDL	1g	201	-	-	X	-
75	CDL	1i	201	-	-	X	-
75	CDL	1q	202	-	-	X	-
75	CDL	3A	501	-	-	X	-
75	CDL	3F	201	-	-	X	-
75	CDL	3N	502	-	-	X	-
75	CDL	3P	513	-	-	X	-
75	CDL	3X	103	-	-	X	-
75	CDL	3Y	106	-	-	X	-
75	CDL	4B	302	-	-	X	-
75	CDL	4C	307	-	-	X	-
76	AYA	1I	203	-	-	X	-
82	PGT	1Y	203	-	-	X	-
91	PGV	4A	609	-	-	X	-
93	PSC	4B	303	-	-	X	-

2 Entry composition

There are 94 unique types of molecules in this entry. The entry contains 124052 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1B	155	Total	C	N	O	S	0	0
			1242	791	226	211	14		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1740	1125	297	316	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	429	Total	C	N	O	S	0	0
			3452	2207	593	628	24		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	174	Total	C	N	O	S	0	0
			1329	892	189	236	12		

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1c	49	Total	C	N	O	S	0	0
			417	276	71	70			

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa].

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1m	128	Total	C	N	O		0	0
			1062	691	182	189			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1o	0	MYR	-	insertion	UNP F1SCH1

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S	0	0
			759	478	143	135	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
45	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 46 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
46	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 47 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
47	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 48 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
48	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 49 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
49	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
49	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 50 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
50	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 51 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
51	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
52	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

- Molecule 53 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3J	56	Total	C	N	O	S	0	0
			464	305	82	77			
53	3W	56	Total	C	N	O	S	0	0
			464	305	82	77			

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
54	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 55 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	4A	514	Total	C	N	O	S	0	0
			4026	2693	625	676	32		

- Molecule 56 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

- Molecule 57 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

- Molecule 58 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 59 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 60 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 61 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 62 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 63 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 64 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 65 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 66 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

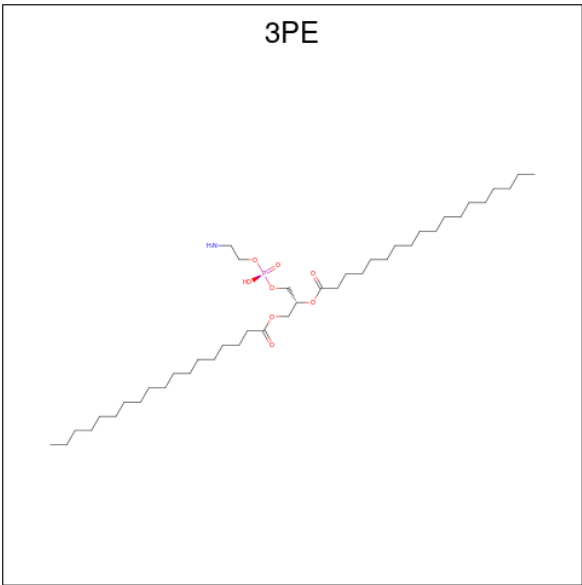
- Molecule 67 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
67	4M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 68 is a protein called Cytochrome c oxidase subunit NDUF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 69 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
69	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1A	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	1B	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1B	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1J	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1J	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1L	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1L	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	1L	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1L	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	1L	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	1L	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1M	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			44	34	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1Z	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1b	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1d	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1d	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	1d	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1e	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1f	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1f	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	1f	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	1f	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	1g	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1g	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	1k	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	1l	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1l	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	1l	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1m	1	Total	C	N	O	P	0
			50	40	1	8	1	
69	1m	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1m	1	Total	C	N	O	P	0
			42	32	1	8	1	
69	1m	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1m	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	1o	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3A	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3C	1	Total	C	N	O	P	0
			35	25	1	8	1	
69	3C	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3C	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	3C	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3D	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	3D	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3E	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3E	1	Total	C	N	O	P	0
			49	39	1	8	1	
69	3G	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			33	23	1	8	1	
69	3G	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3G	1	Total	C	N	O	P	0
			43	33	1	8	1	
69	3G	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3J	1	Total	C	N	O	P	0
			47	37	1	8	1	
69	3J	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	3J	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3J	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3J	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3N	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			38	28	1	8	1	
69	3P	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	

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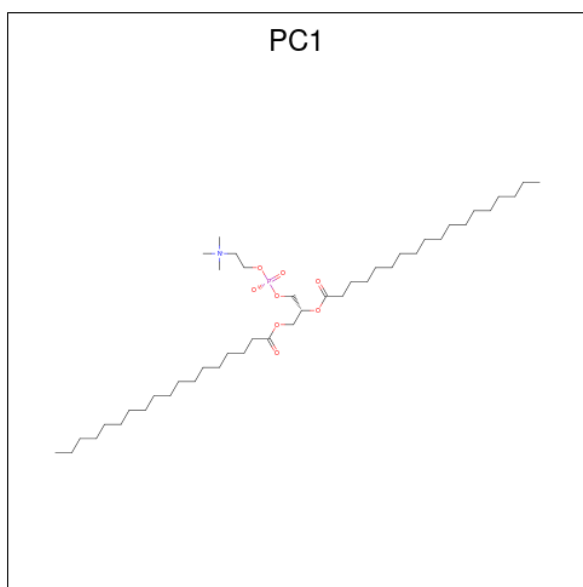
Mol	Chain	Residues	Atoms					AltConf
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3P	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3P	1	Total	C	N	O	P	0
			48	38	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3P	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Q	1	Total	C	N	O	P	0
			41	31	1	8	1	
69	3Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	3Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
69	3R	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3R	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3R	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3S	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3T	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3W	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3W	1	Total	C	N	O	P	0
			42	32	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
69	3W	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3X	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			45	35	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	3Y	1	Total	C	N	O	P	0
			51	41	1	8	1	
69	4G	1	Total	C	N	O	P	0
			32	22	1	8	1	
69	4G	1	Total	C	N	O	P	0
			41	31	1	8	1	

- Molecule 70 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



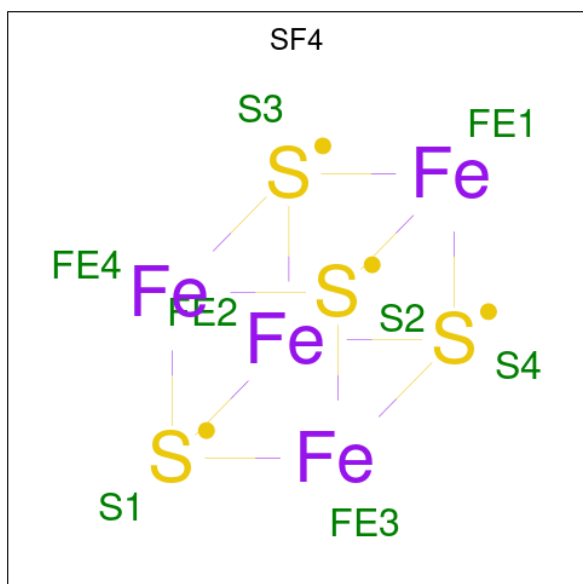
Mol	Chain	Residues	Atoms					AltConf
70	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1B	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1H	1	Total	C	N	O	P	0
			48	38	1	8	1	
70	1H	1	Total	C	N	O	P	0
			41	31	1	8	1	
70	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
70	1P	1	Total	C	N	O	P	0
			33	23	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	1Y	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
70	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
70	1h	1	Total	C	N	O	P	0
			46	36	1	8	1	
70	3J	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3P	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3R	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3T	1	Total	C	N	O	P	0
			54	44	1	8	1	
70	3X	1	Total	C	N	O	P	0
			54	44	1	8	1	

- Molecule 71 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



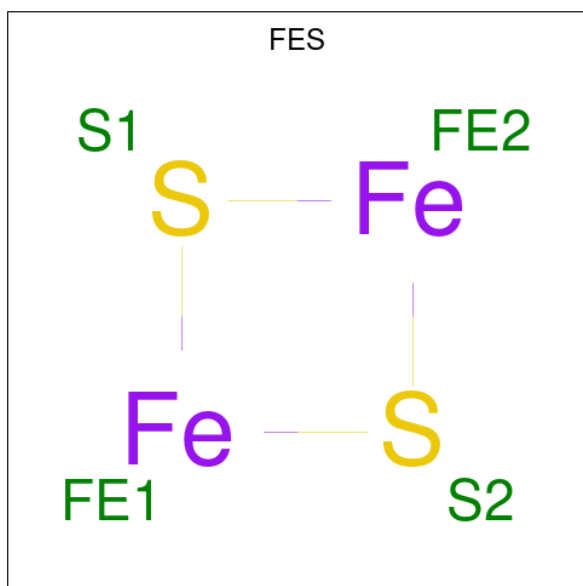
Mol	Chain	Residues	Atoms			AltConf
71	1B	1	Total	Fe	S	0
			8	4	4	
71	1F	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1G	1	Total	Fe	S	0
			8	4	4	
71	1I	1	Total	Fe	S	0
			8	4	4	

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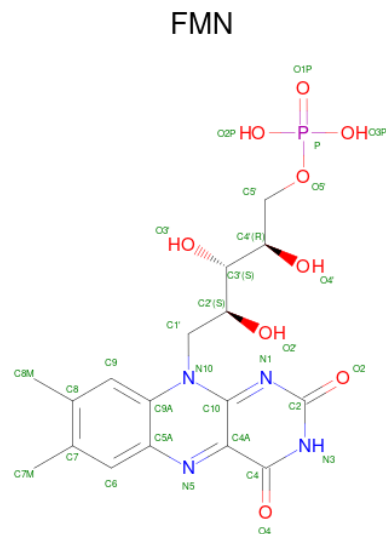
Mol	Chain	Residues	Atoms			AltConf
71	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 72 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
72	1E	1	Total	Fe	S	0
			4	2	2	
72	1G	1	Total	Fe	S	0
			4	2	2	
72	3E	1	Total	Fe	S	0
			4	2	2	
72	3R	1	Total	Fe	S	0
			4	2	2	

- Molecule 73 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

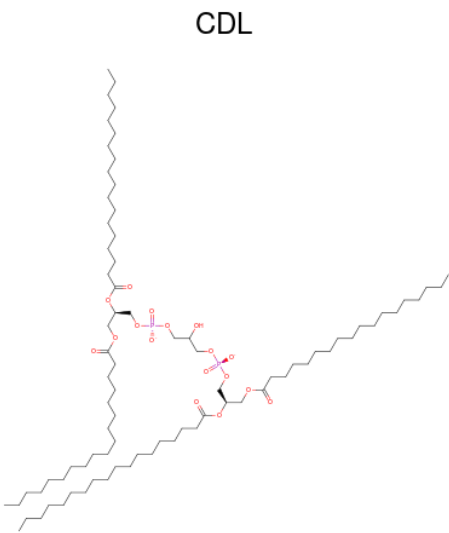


Mol	Chain	Residues	Atoms					AltConf
73	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 74 is POTASSIUM ION (CCD ID: K) (formula: K).

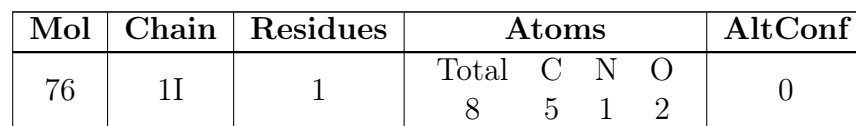
Mol	Chain	Residues	Atoms	AltConf
74	1G	1	Total K 1 1	0

- Molecule 75 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



Mol	Chain	Residues	Atoms				AltConf
75	1H	1	Total	C	O	P	0
			51	32	17	2	
75	1L	1	Total	C	O	P	0
			87	68	17	2	
75	1N	1	Total	C	O	P	0
			77	58	17	2	
75	1Y	1	Total	C	O	P	0
			100	81	17	2	
75	1d	1	Total	C	O	P	0
			86	67	17	2	
75	1d	1	Total	C	O	P	0
			93	74	17	2	
75	1g	1	Total	C	O	P	0
			100	81	17	2	
75	1i	1	Total	C	O	P	0
			80	61	17	2	
75	1q	1	Total	C	O	P	0
			61	42	17	2	
75	1q	1	Total	C	O	P	0
			100	81	17	2	
75	3A	1	Total	C	O	P	0
			98	79	17	2	
75	3D	1	Total	C	O	P	0
			56	37	17	2	
75	3F	1	Total	C	O	P	0
			100	81	17	2	
75	3N	1	Total	C	O	P	0
			100	81	17	2	
75	3P	1	Total	C	O	P	0
			100	81	17	2	
75	3T	1	Total	C	O	P	0
			57	38	17	2	
75	3X	1	Total	C	O	P	0
			100	81	17	2	
75	3Y	1	Total	C	O	P	0
			100	81	17	2	
75	4B	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	
75	4C	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 76 is N-ACETYLALANINE (CCD ID: AYA) (formula: $C_5H_9NO_3$).



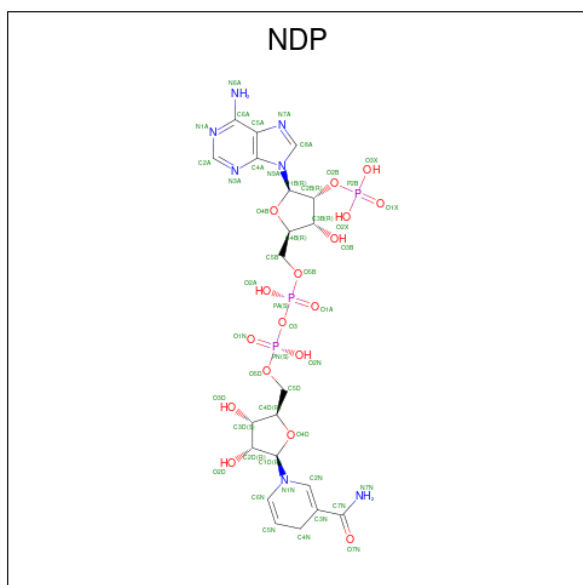
-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar, which is in turn linked to a chain of three phosphate groups. The structure is color-coded: the guanine base is blue, the ribose sugar is green, and the phosphate groups are pink. Atoms are labeled with their respective element symbols and numbers (e.g., N1, N3, N7, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O807, O808, O809, O810, O811, O

Mol	Chain	Residues	Atoms					AltConf
77	1O	1	Total 32	C 10	N 5	O 14	P 3	0

- 

Mol	Chain	Residues	Atoms		AltConf
78	1O	1	Total	Mg	0
			1	1	
78	4A	1	Total	Mg	0
			1	1	

- Molecule 79 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

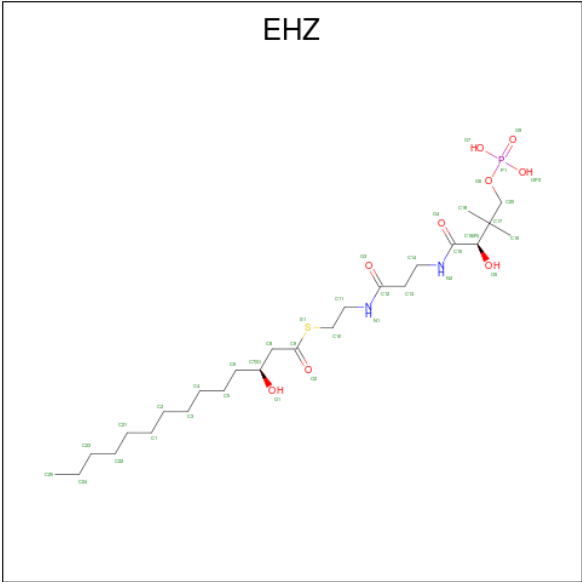


Mol	Chain	Residues	Atoms					AltConf
79	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 80 is ZINC ION (CCD ID: ZN) (formula: Zn).

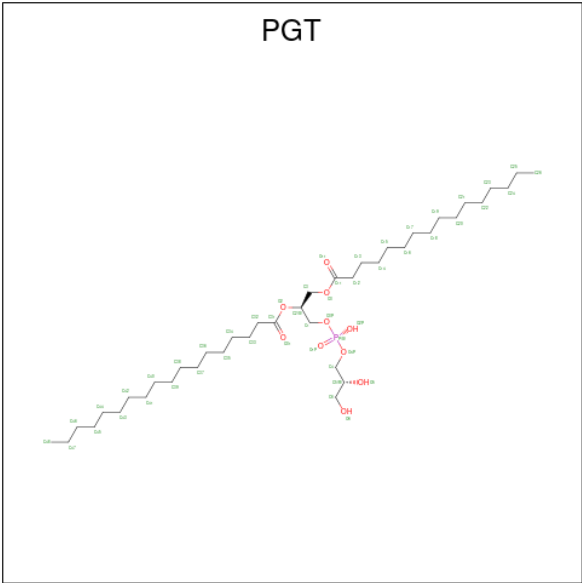
Mol	Chain	Residues	Atoms		AltConf
80	1R	1	Total	Zn	0
			1	1	
80	4F	1	Total	Zn	0
			1	1	

- Molecule 81 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



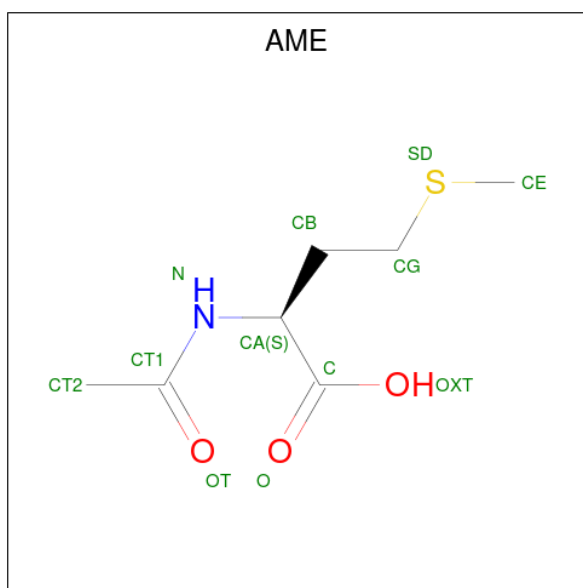
Mol	Chain	Residues	Atoms						AltConf
81	1T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
81	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 82 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



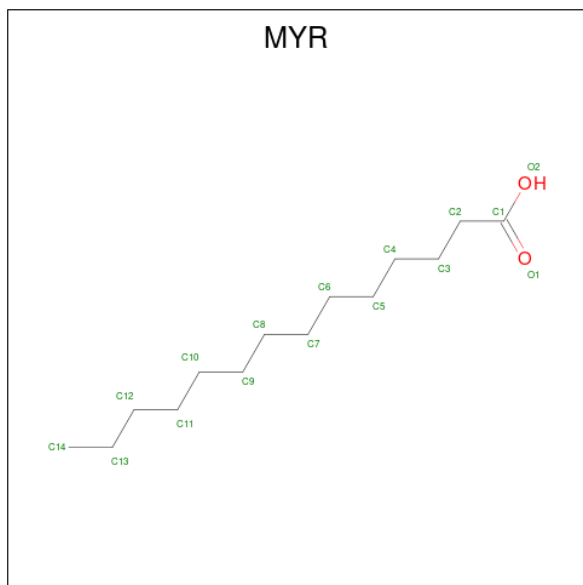
Mol	Chain	Residues	Atoms				AltConf
82	1Y	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 83 is N-ACETYL METHIONINE (CCD ID: AME) (formula: $C_7H_{13}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
83	1h	1	11	7	1	2	1	0

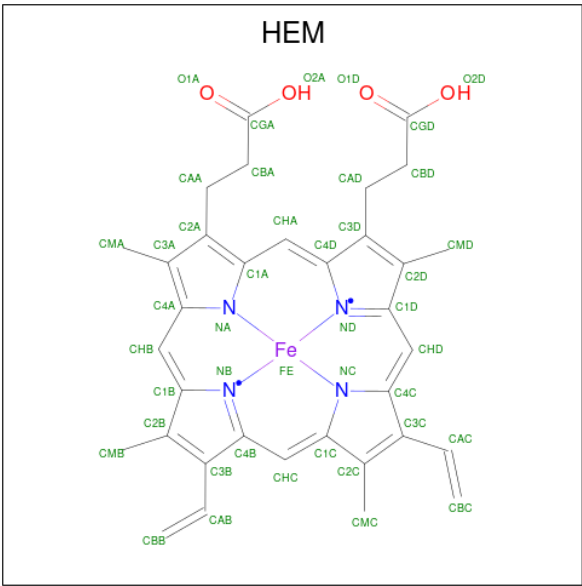
- Molecule 84 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
84	1l	1	15	14	1	0

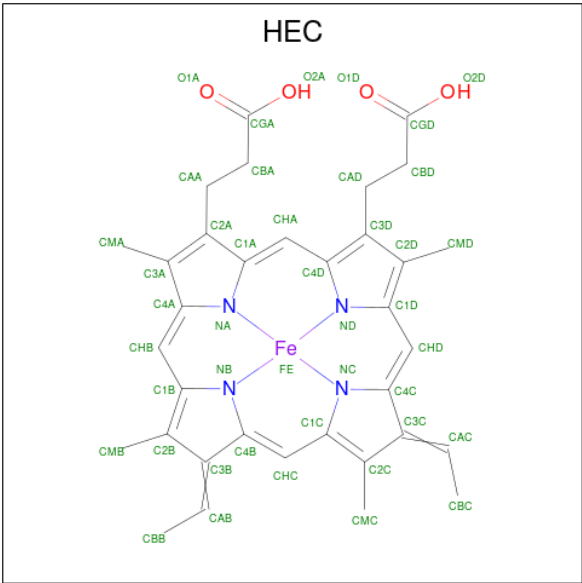
- Molecule 85 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



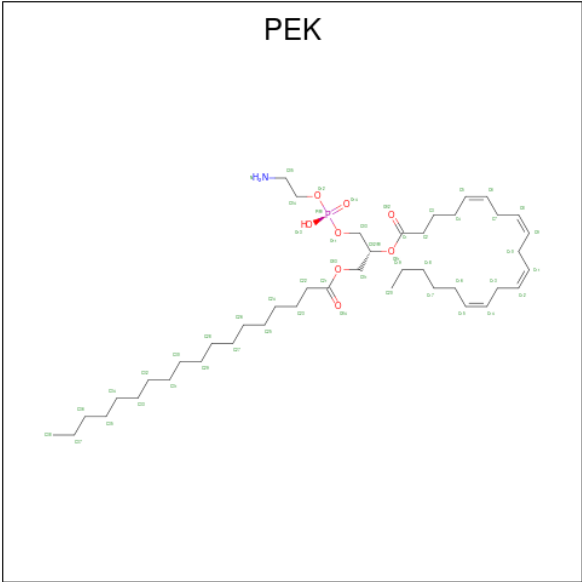
Mol	Chain	Residues	Atoms					AltConf
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3C	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0
85	3P	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 86 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



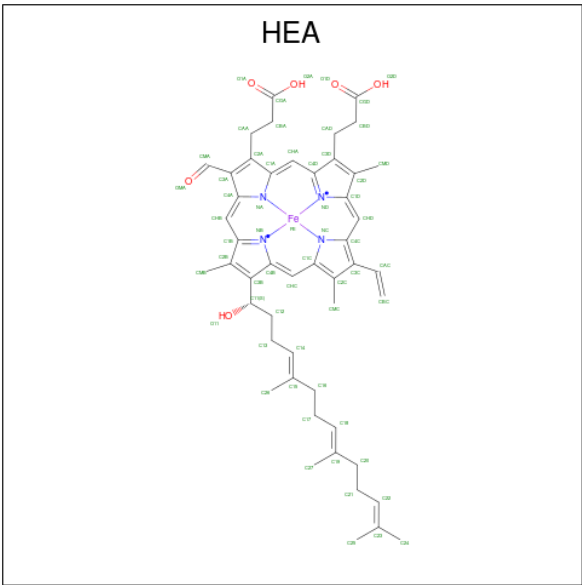
Mol	Chain	Residues	Atoms					AltConf
86	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
86	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 87 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
87	3X	1	Total	C	N	O	P	0
			53	43	1	8	1	
87	4G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 88 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0
88	4A	1	Total 60	C 49	Fe 1	N 4	O 6	0

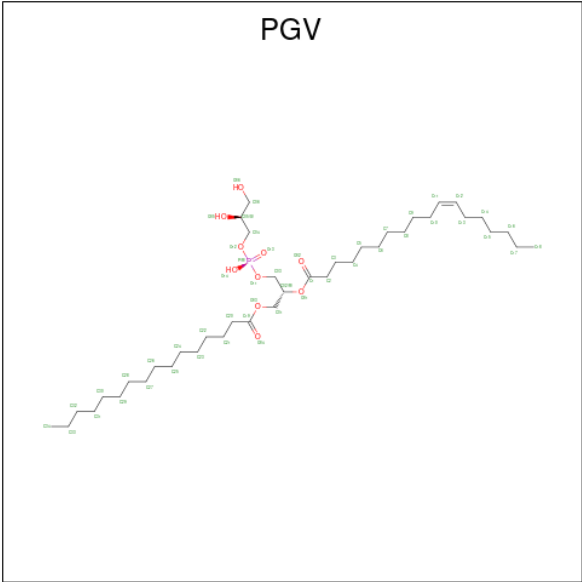
- Molecule 89 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
89	4A	1	Total	Cu	0
			1	1	

- Molecule 90 is SODIUM ION (CCD ID: NA) (formula: Na).

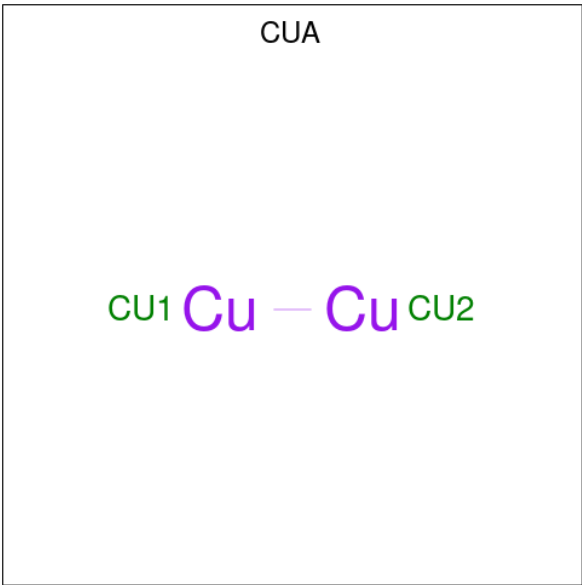
Mol	Chain	Residues	Atoms		AltConf
90	4A	1	Total	Na	0
			1	1	

- Molecule 91 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



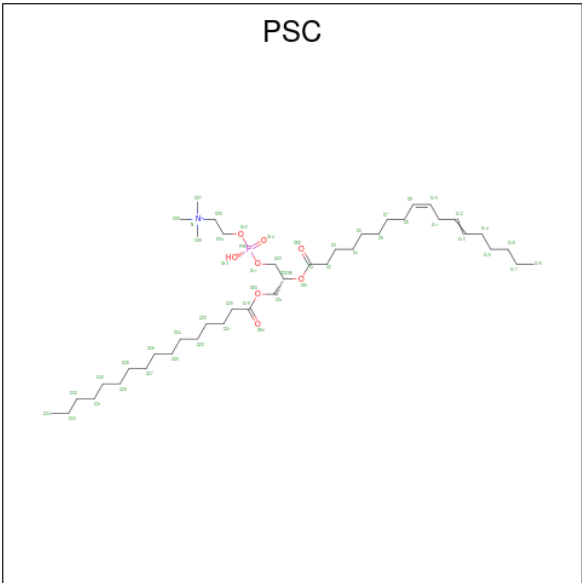
Mol	Chain	Residues	Atoms				AltConf
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4A	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4C	1	Total	C	O	P	0
			51	40	10	1	
91	4G	1	Total	C	O	P	0
			51	40	10	1	
91	4J	1	Total	C	O	P	0
			42	31	10	1	
91	4K	1	Total	C	O	P	0
			43	32	10	1	
91	4N	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 92 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



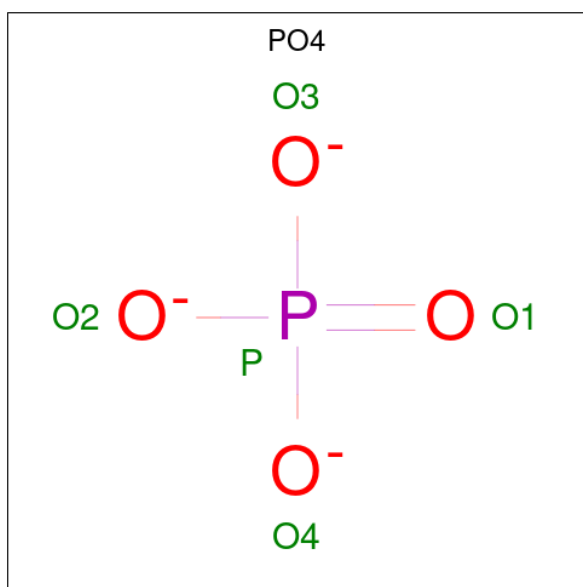
Mol	Chain	Residues	Atoms		AltConf
92	4B	1	Total	Cu	0
			2	2	

- Molecule 93 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms					AltConf
93	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 94 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

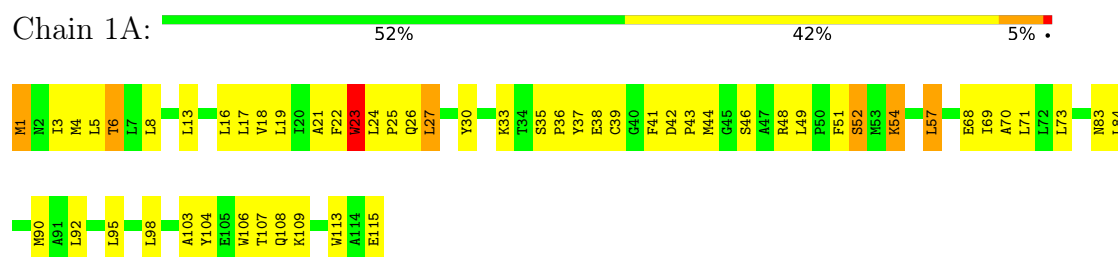


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
94	4H	1	5	4	1	0

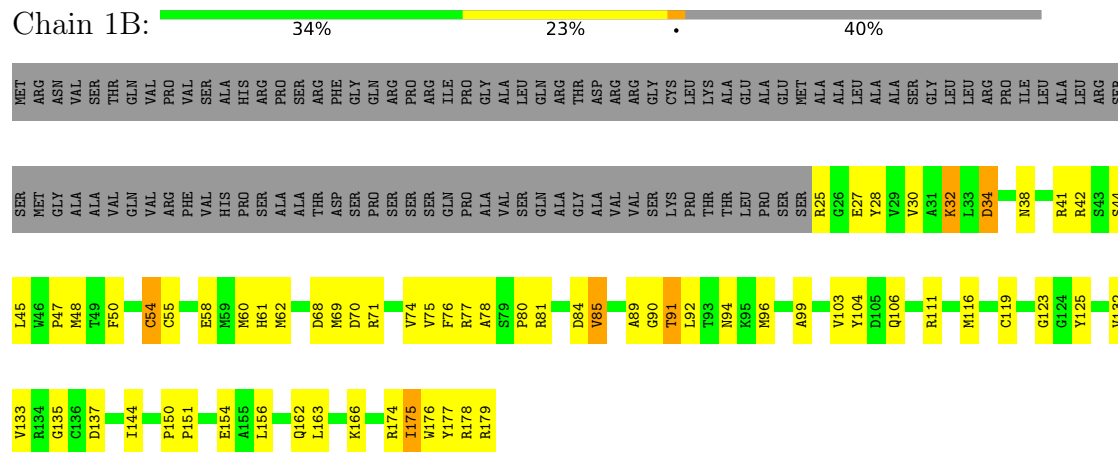
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

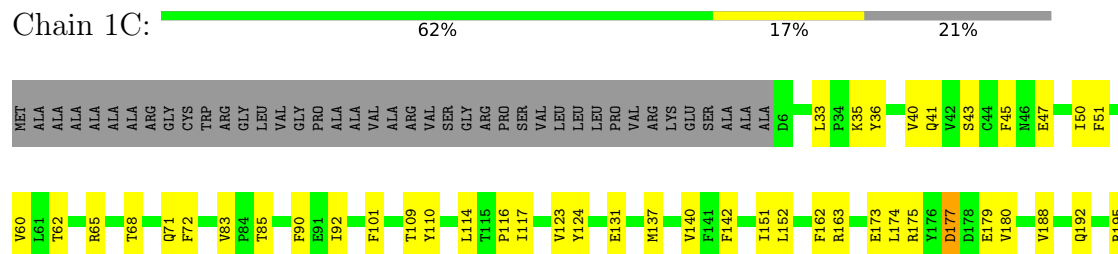
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

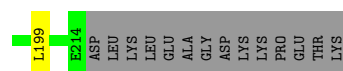


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



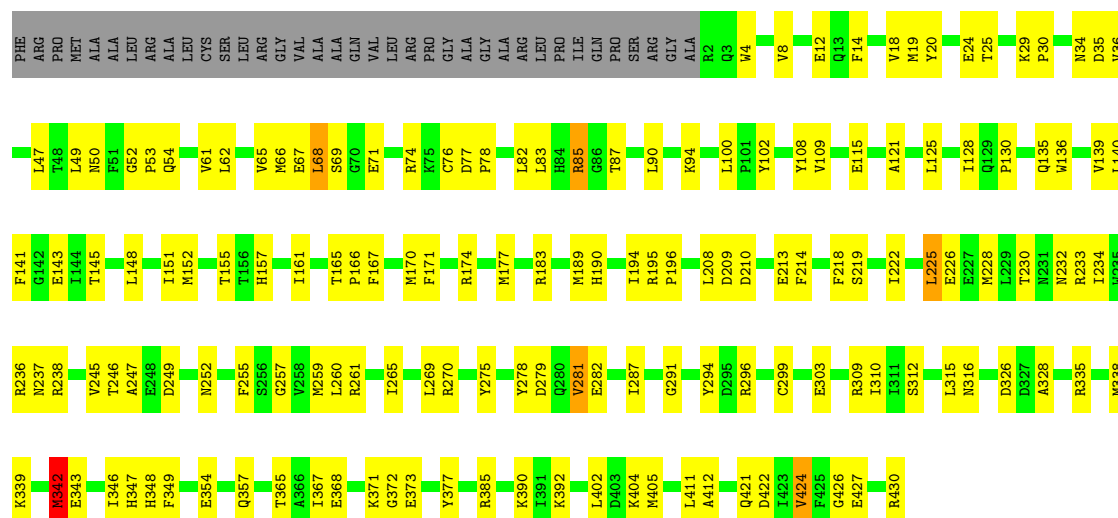
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial





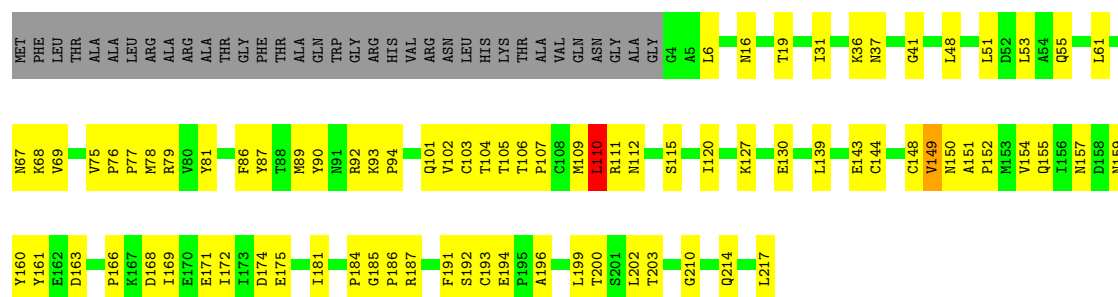
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D: 59% 32% 8%



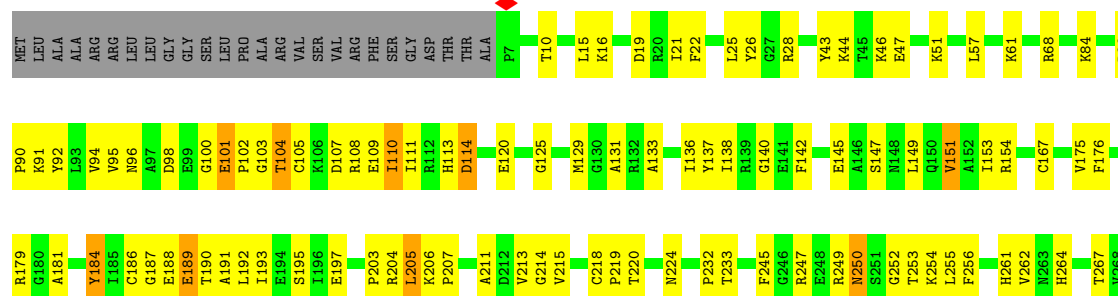
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

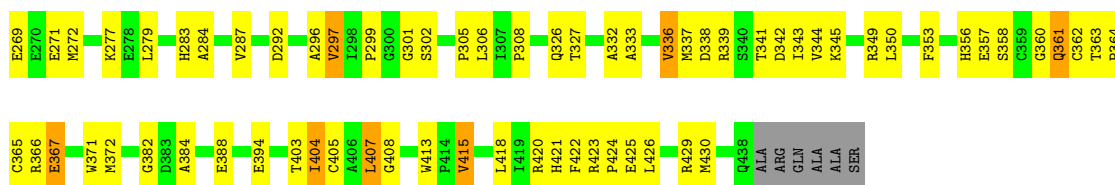
Chain 1E: 53% 32% 14%



- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

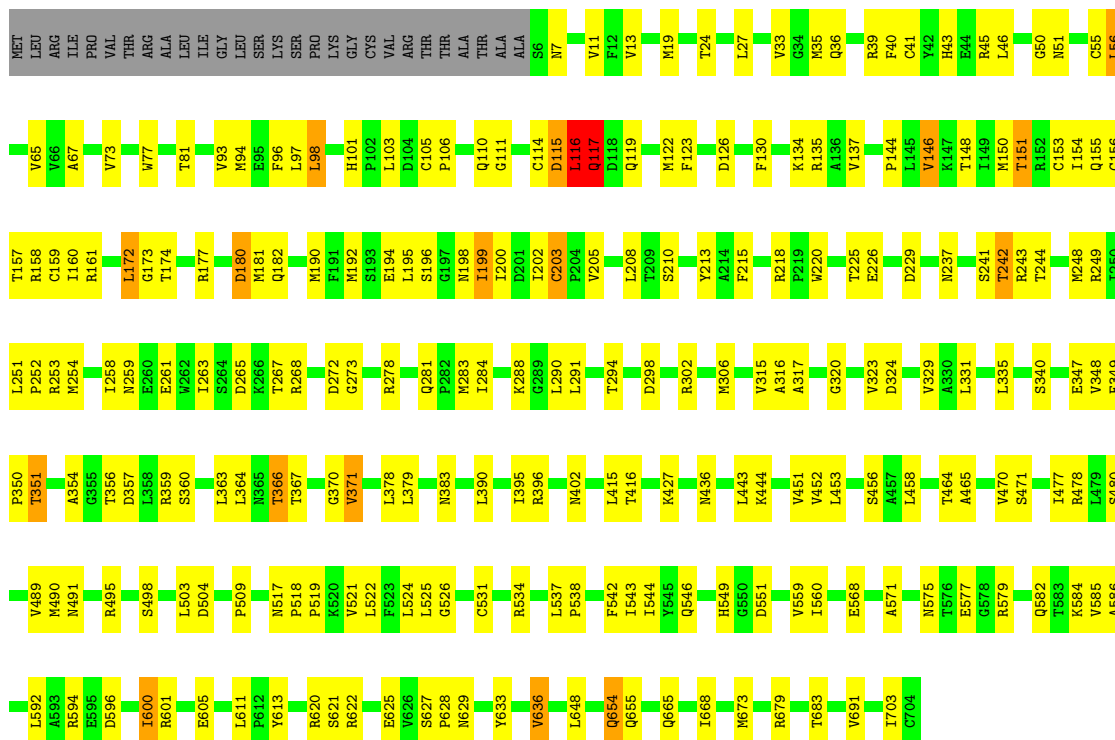
Chain 1F: 57% 32% 7%





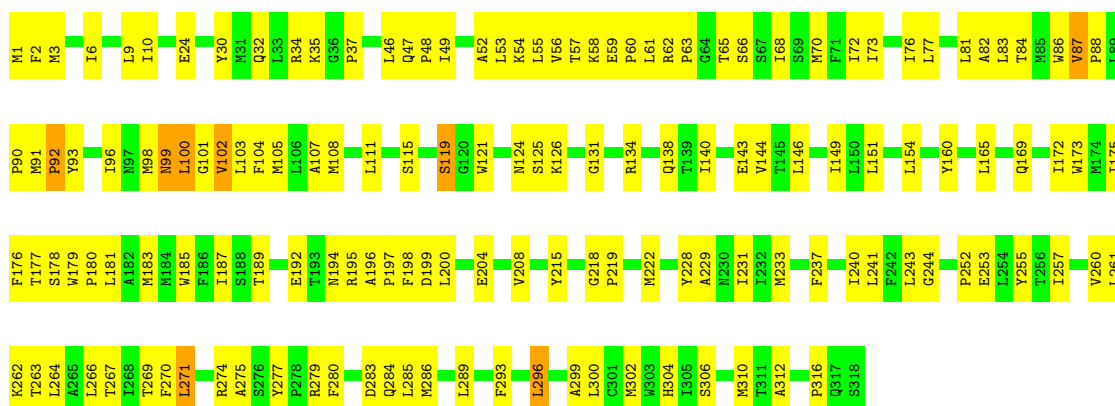
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G: 64% 30%

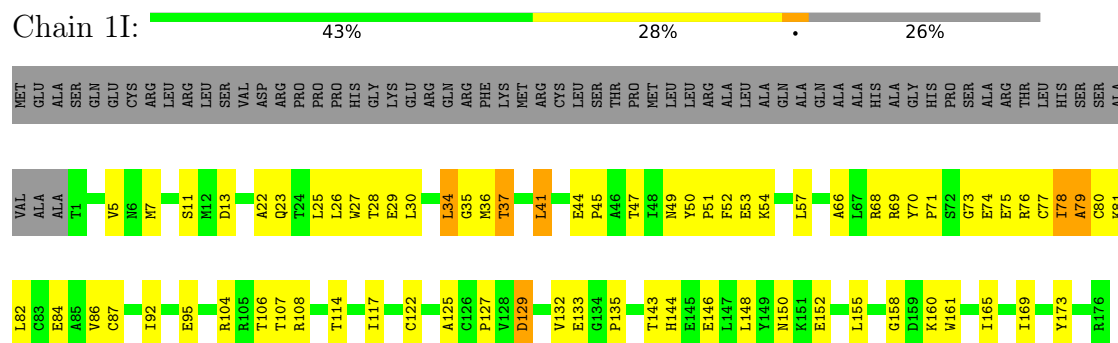


- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

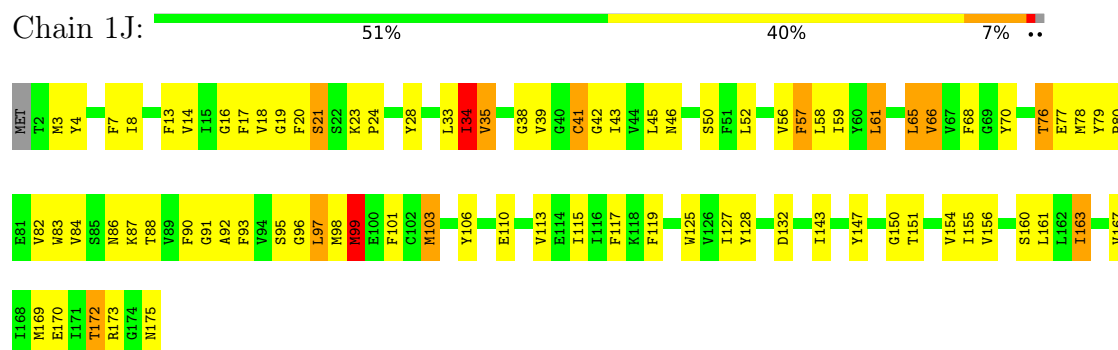
Chain 1H: 53% 44%



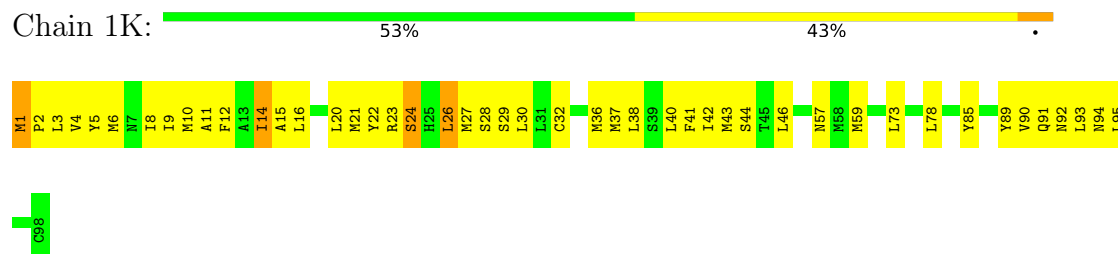
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



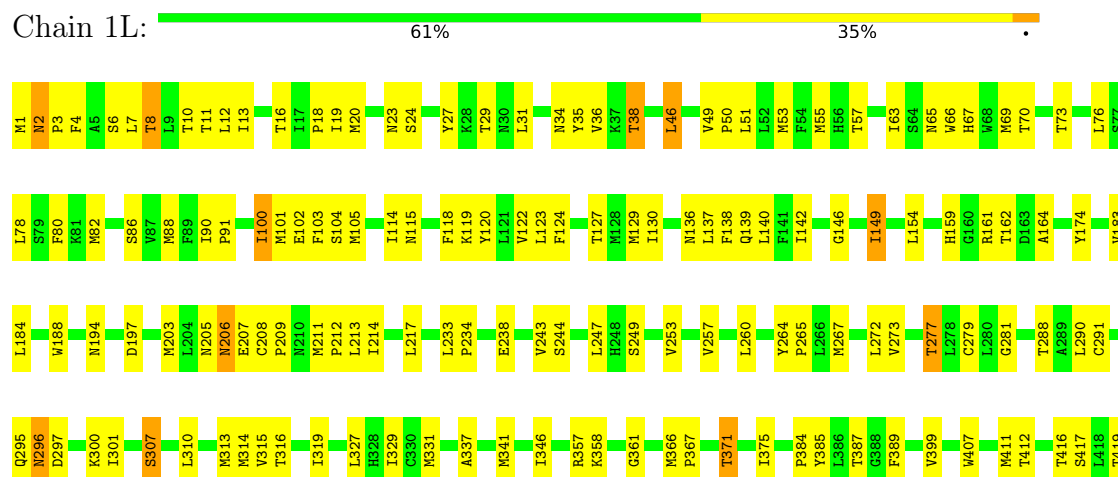
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



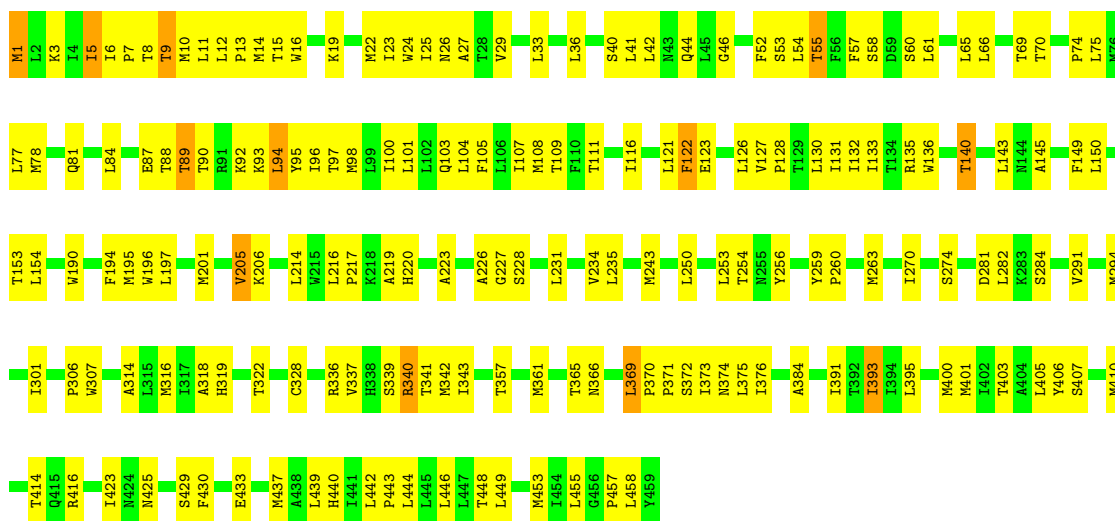
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5





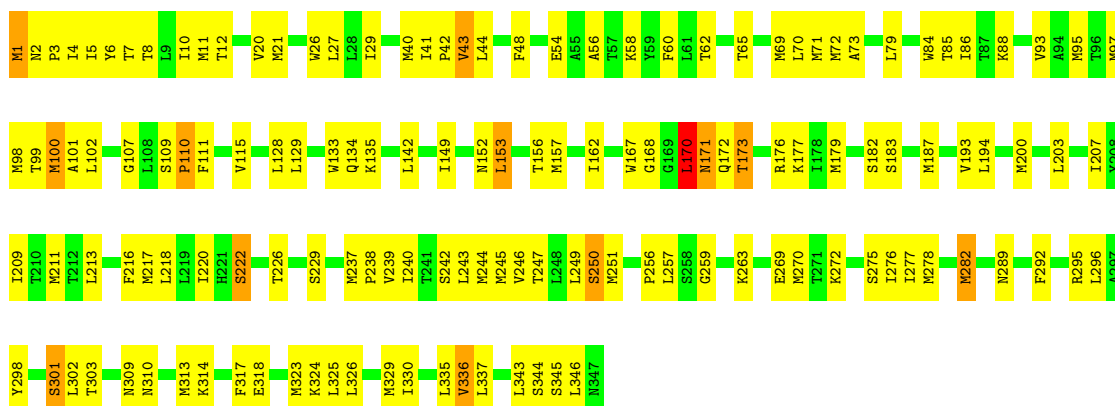
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M: 61% 37% .



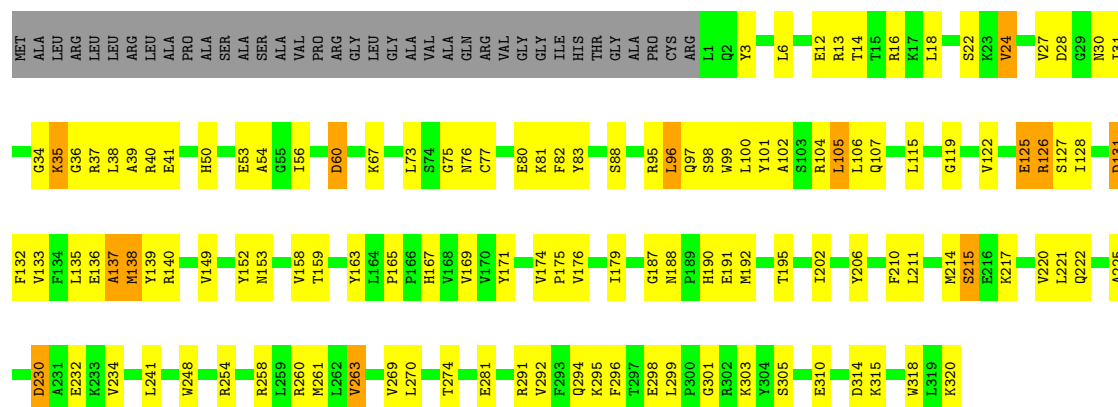
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain 1N: 59% 37% .



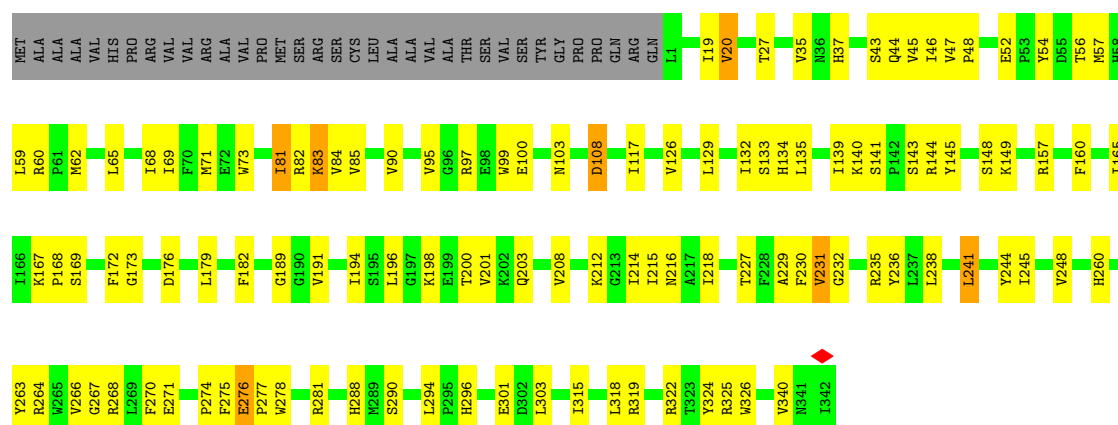
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain 1O: 55% 31% 10% .



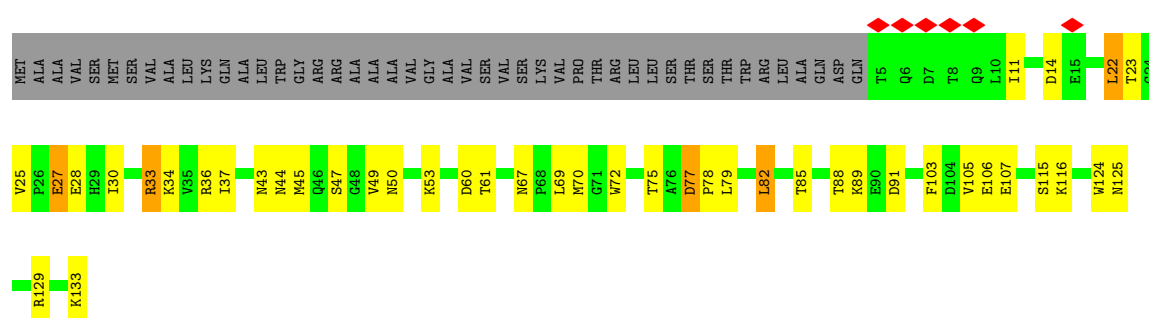
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P: 60% 29% 9%



• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

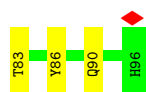
Chain 1Q: 49% 22% 26%



• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R: 63% 15% 22%





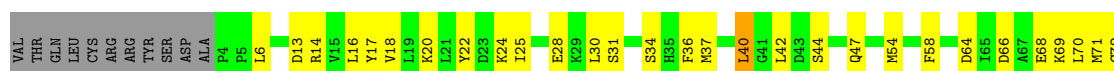
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S: 62% 23% 12%



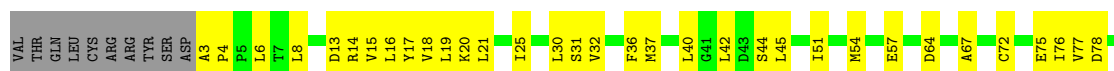
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T: 31% 23% 46%



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U: 32% 23% 45%



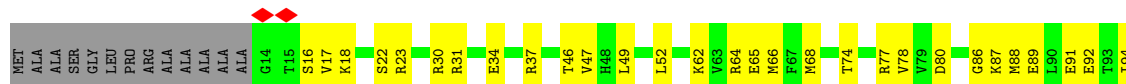
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V: 74% 22%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

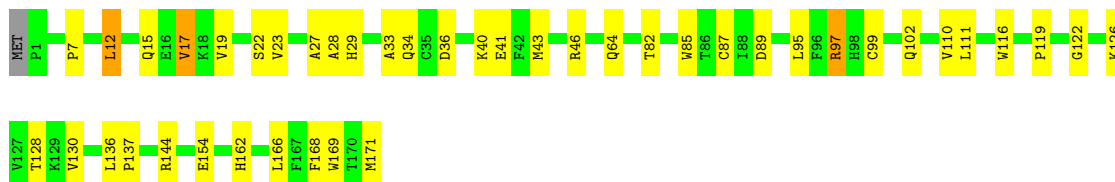
Chain 1W: 64% 25% 10%





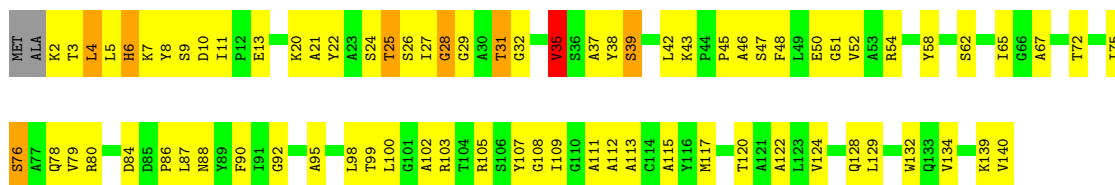
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain 1X: 74% 23% ..



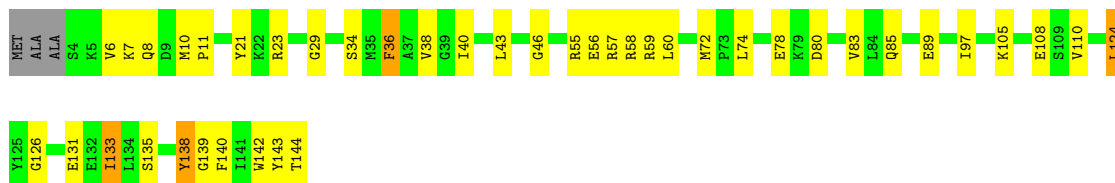
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: 45% 48% 5% ..



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z: 69% 26% ..



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a: 64% 34% .

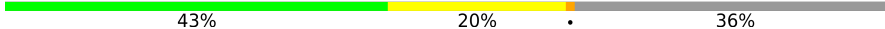


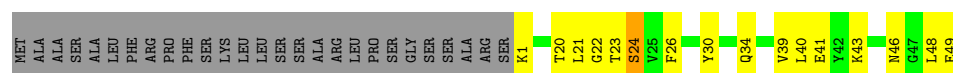
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b: 71% 25% ..



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c: 



- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d: 



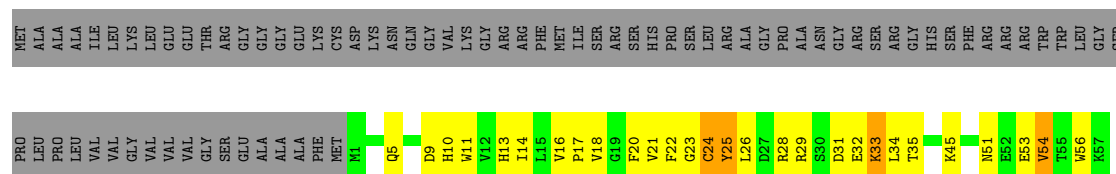
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e: 



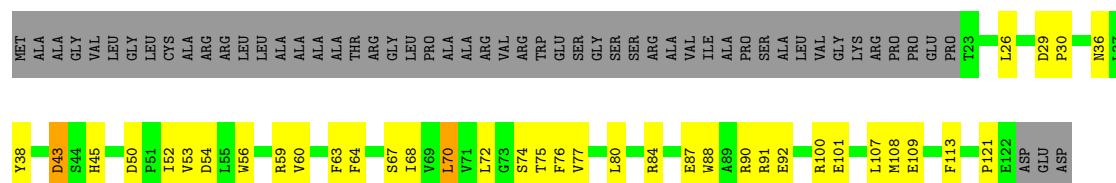
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f: 



- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

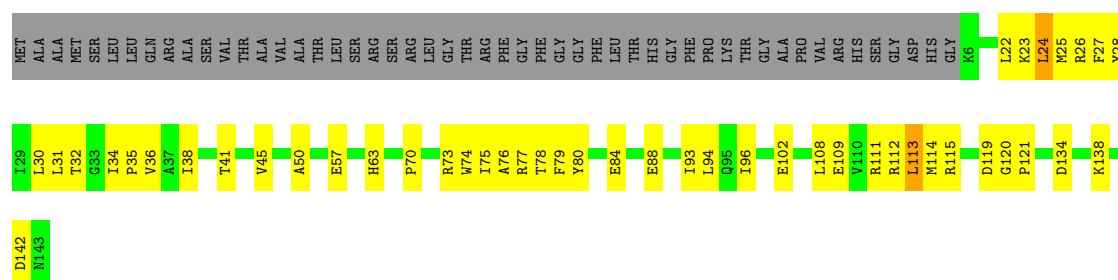
Chain 1g: 



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

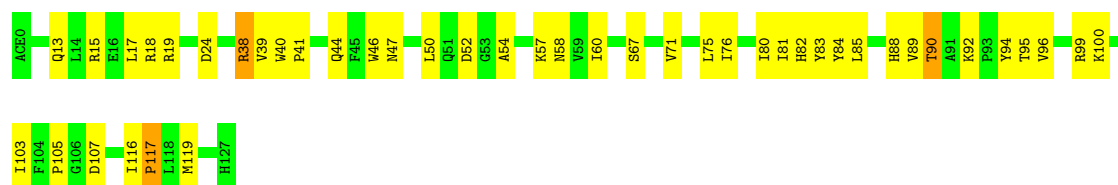
Chain 1h: 





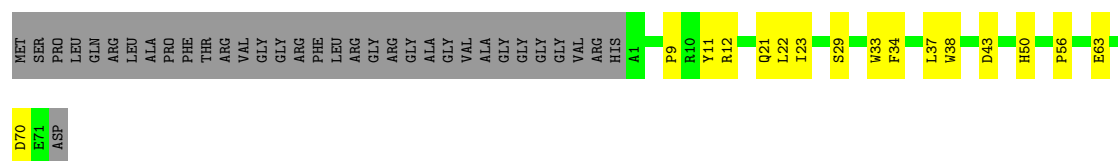
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i: 66% 32% .



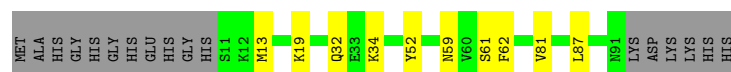
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j: 52% 15% 32%



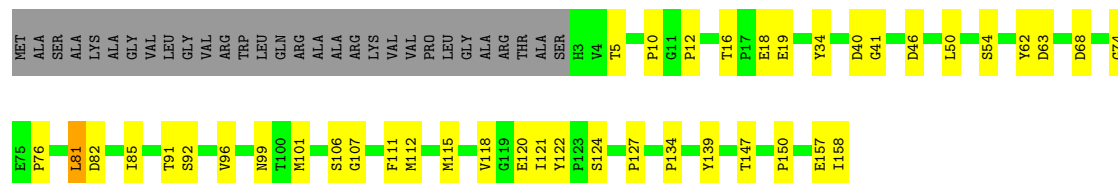
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k: 72% 10% 17%



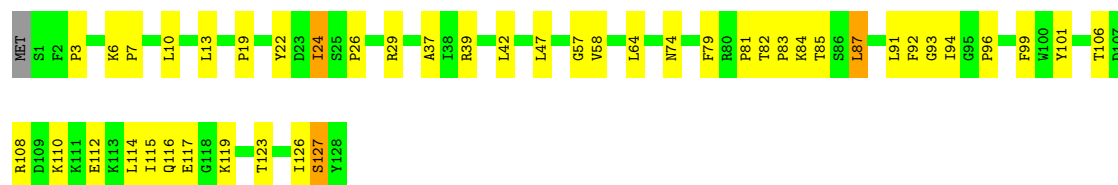
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l: 61% 22% 16%



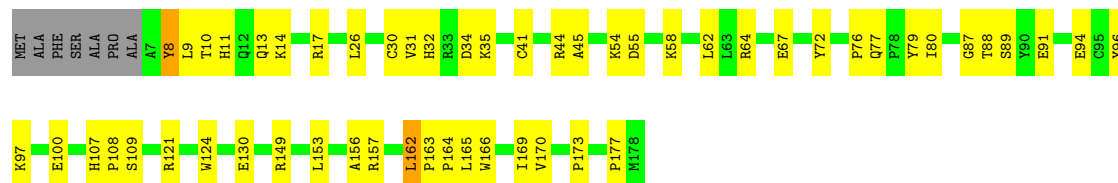
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 65% 32% ..



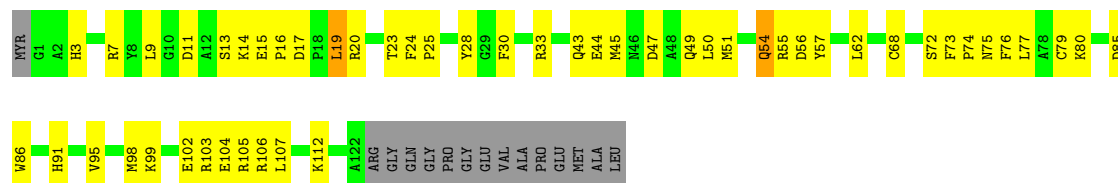
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 66% 29% . .



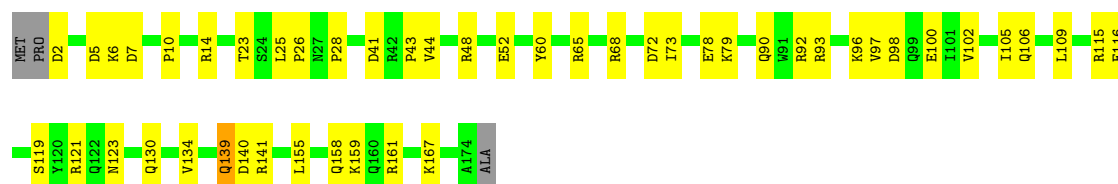
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o: 52% 36% . 11%



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p: 71% 27% . .



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

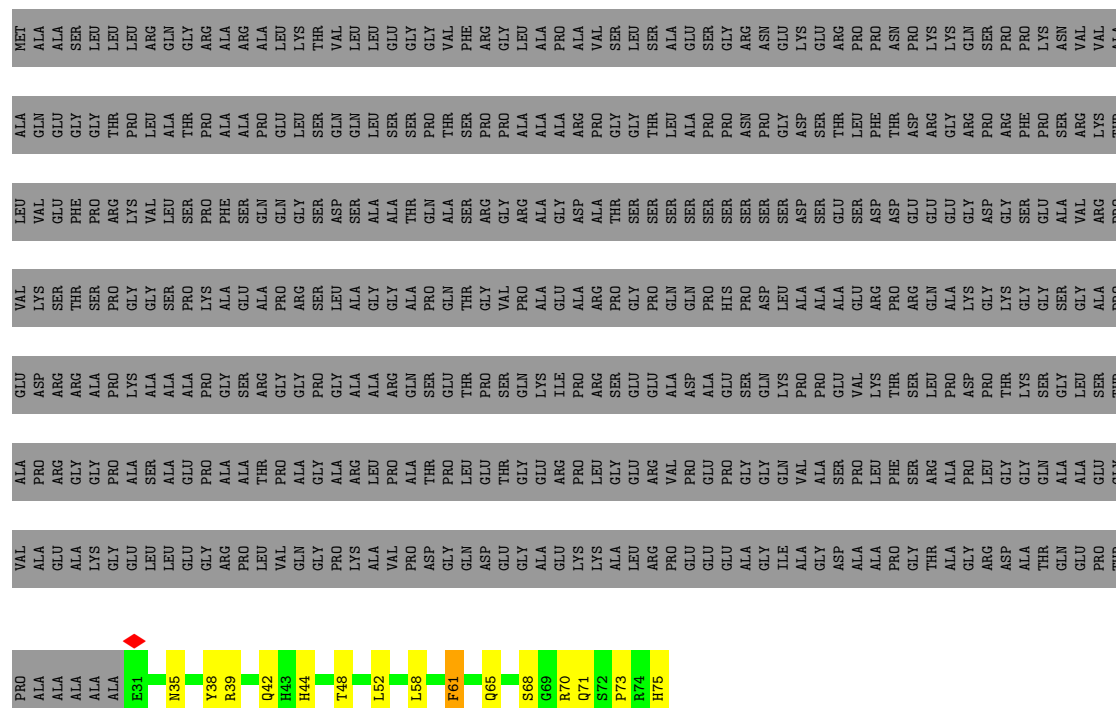
Chain 1q: 73% 26% .



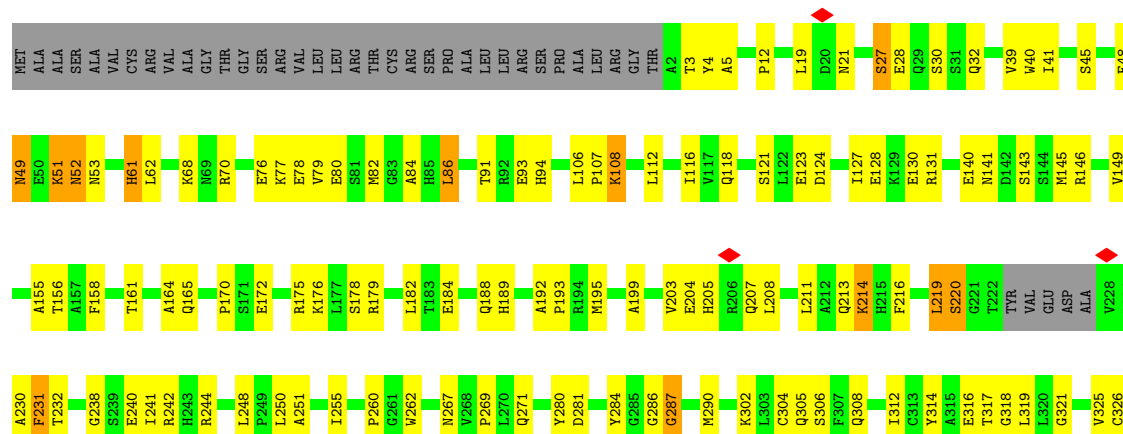
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

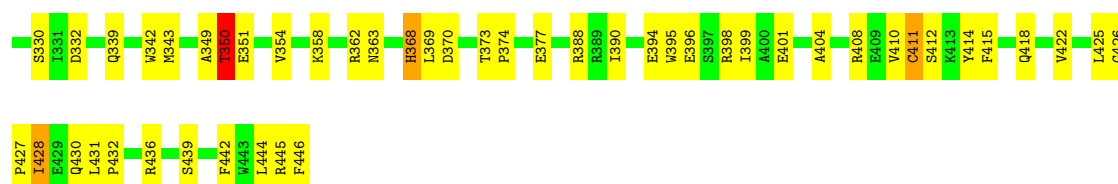


Chain 1s: 6% 90%



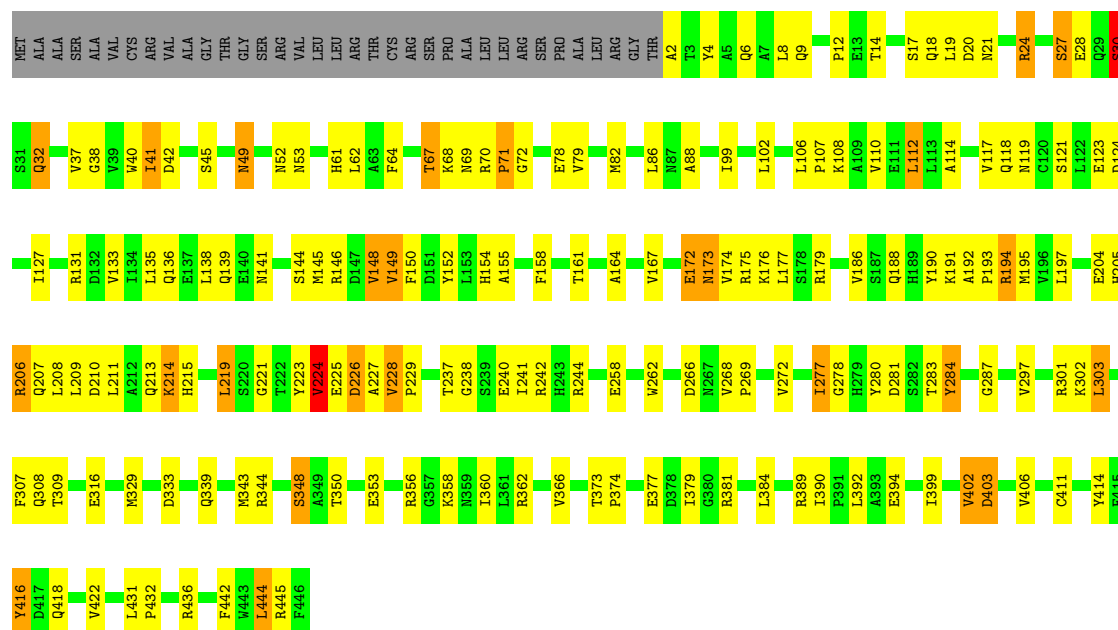
Chain 3A: 56% 32% 8%





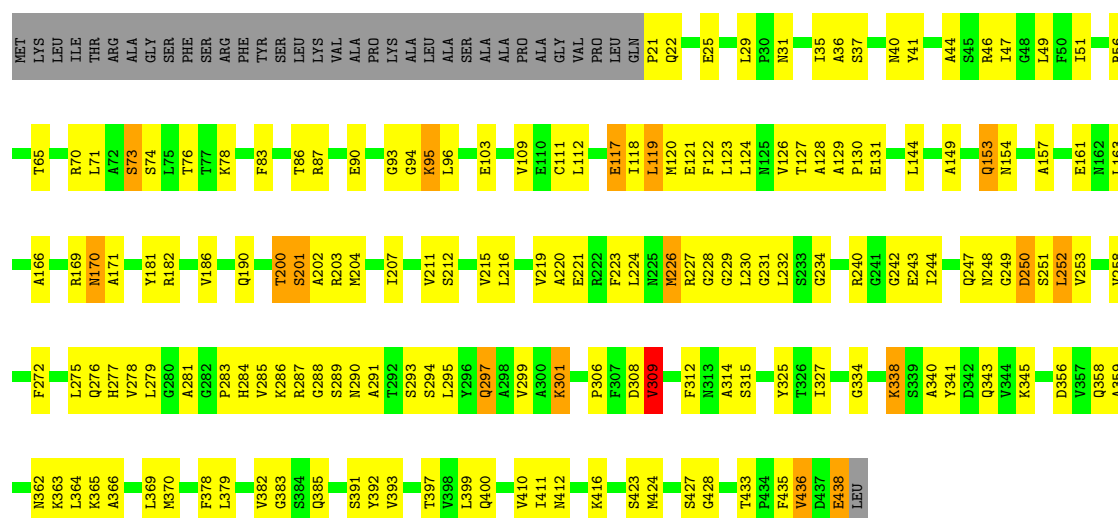
- Molecule 45: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain 3N: 56% 31% 5% 7%



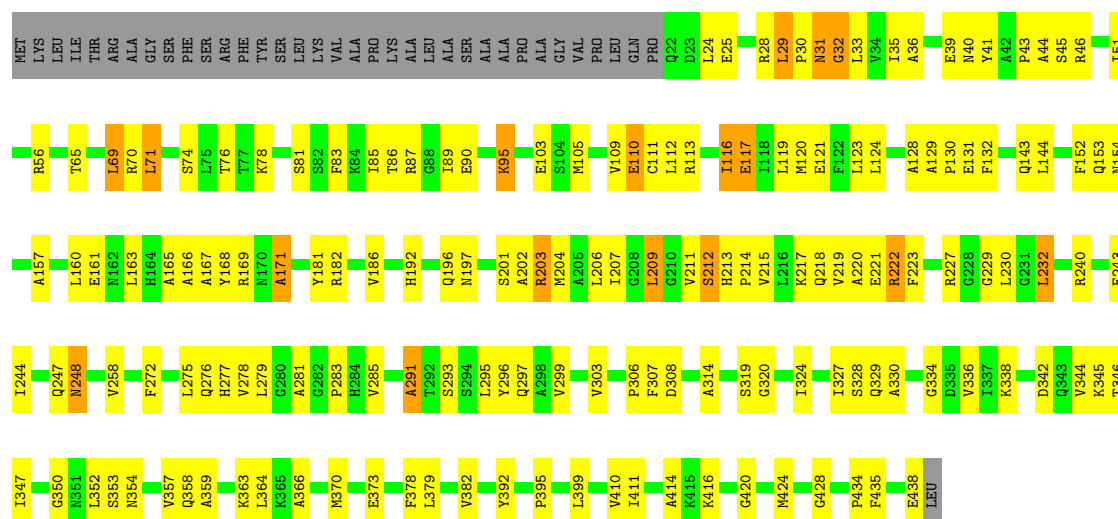
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3B: 55% 33% 8%



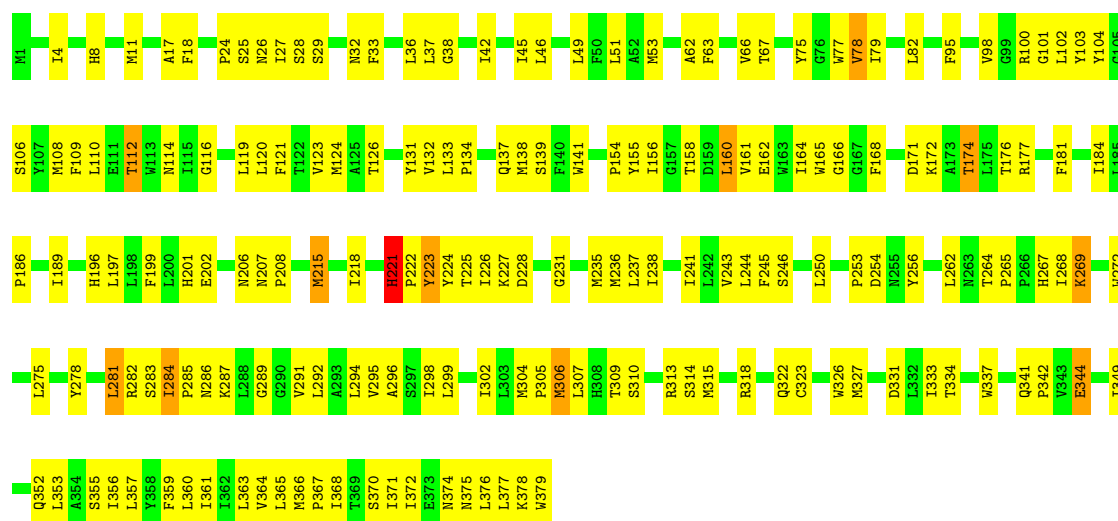
- Molecule 46: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain 3O:  55% 33% 8%



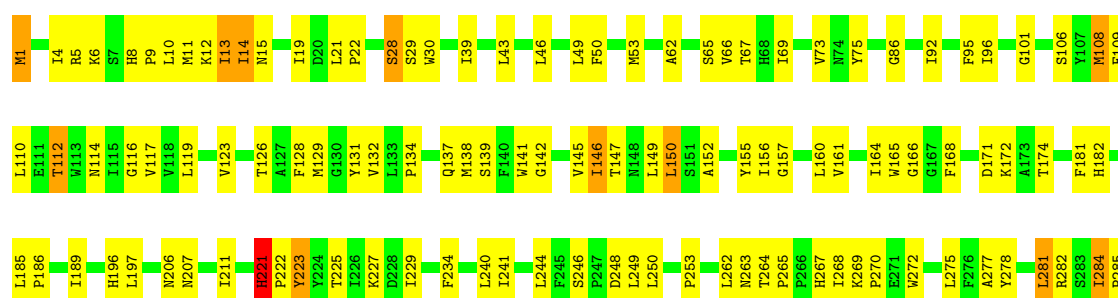
• Molecule 47: Cytochrome b

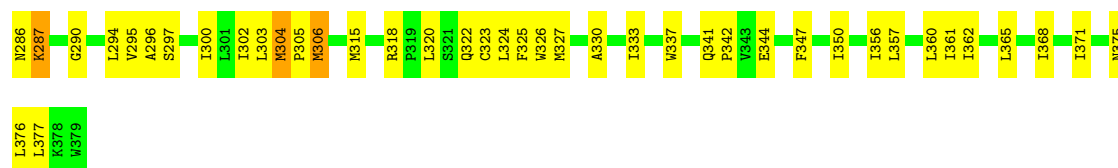
Chain 3C:  52% 45%



• Molecule 47: Cytochrome b

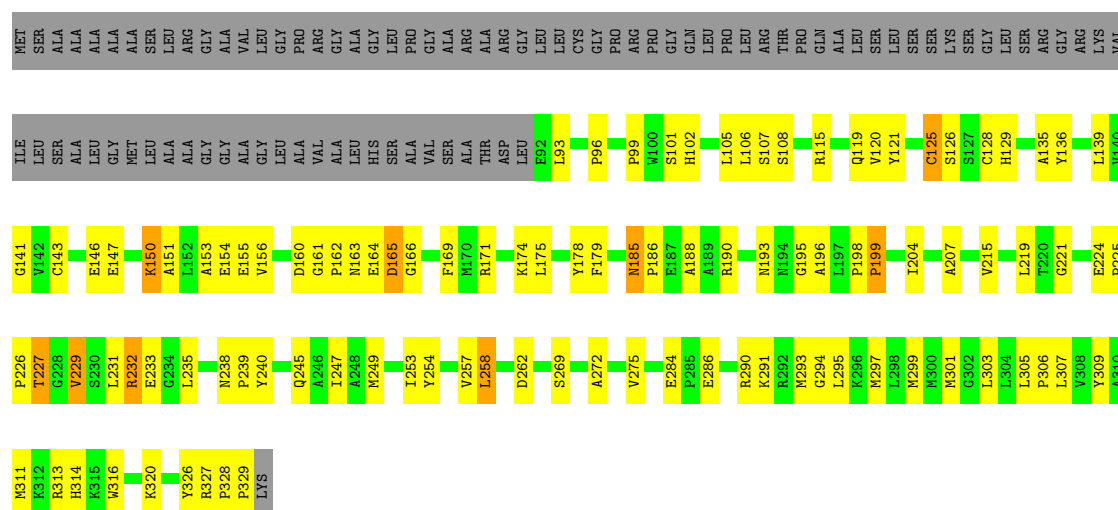
Chain 3P:  59% 37%





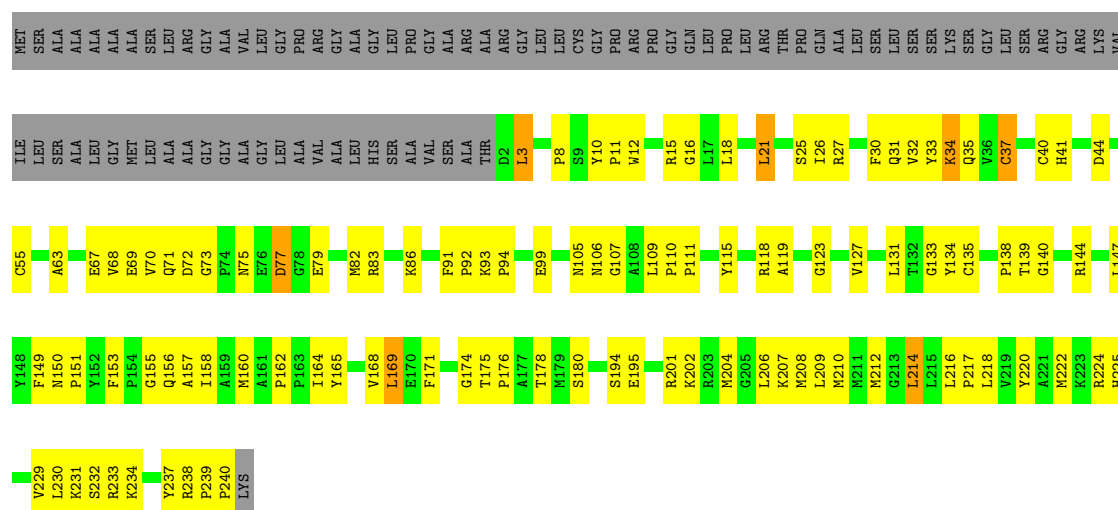
• Molecule 48: Cytochrome c1

Chain 3D: 41% 29% 27%



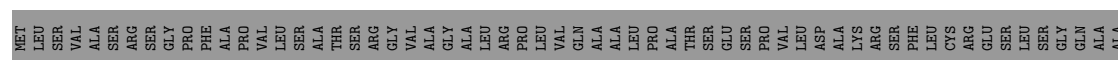
• Molecule 48: Cytochrome c1

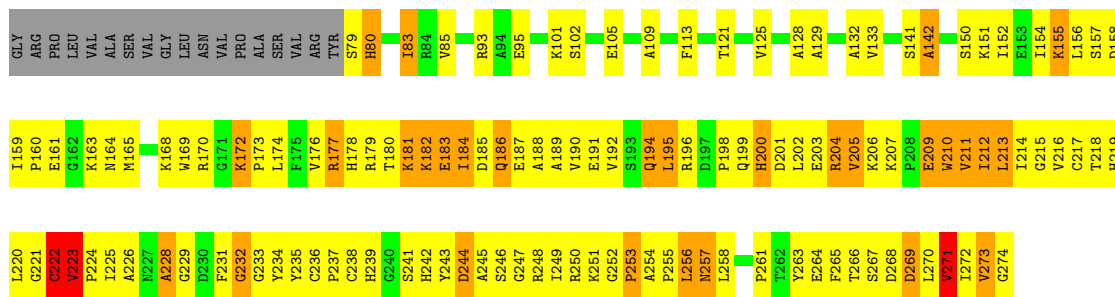
Chain 3Q: 39% 32% 27%



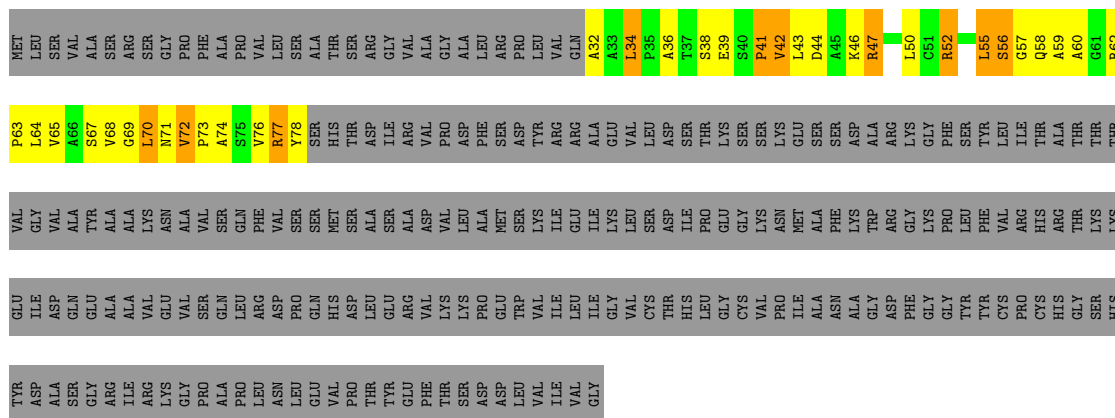
• Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 3E: 24% 35% 11% 28%

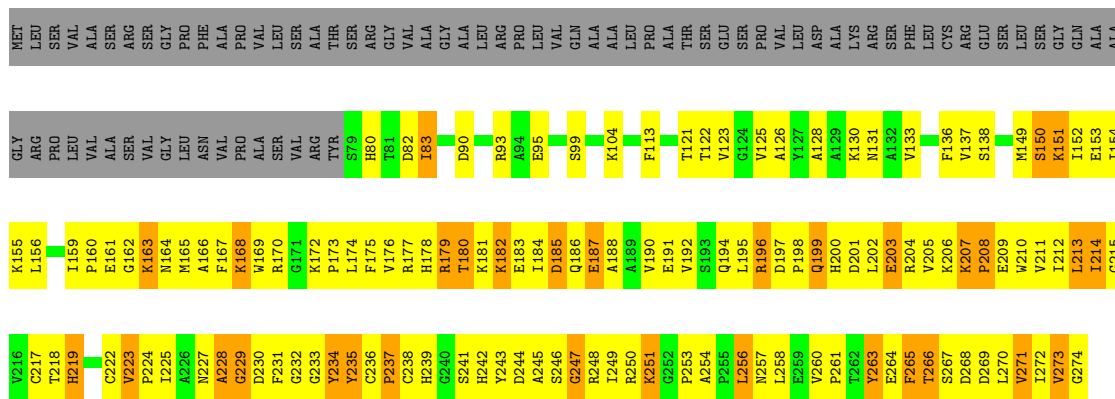
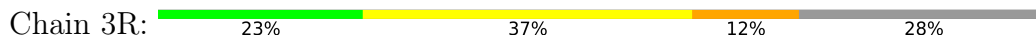




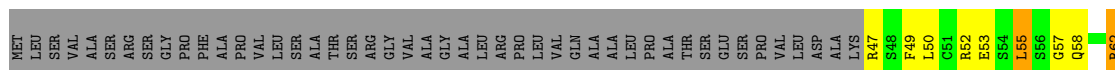
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial

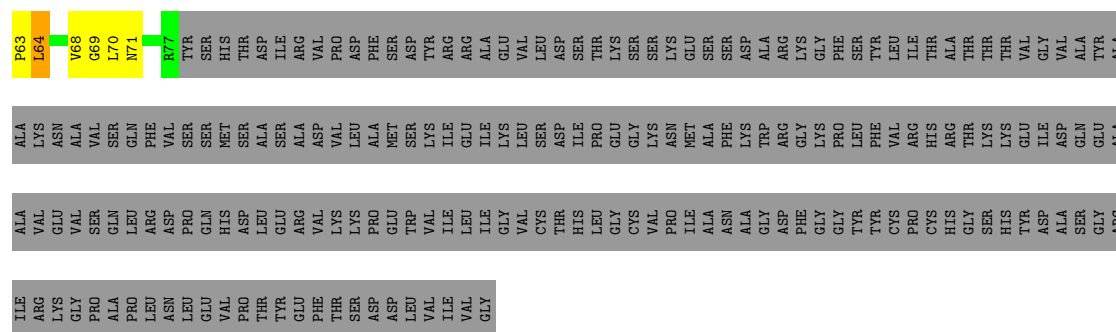


- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial



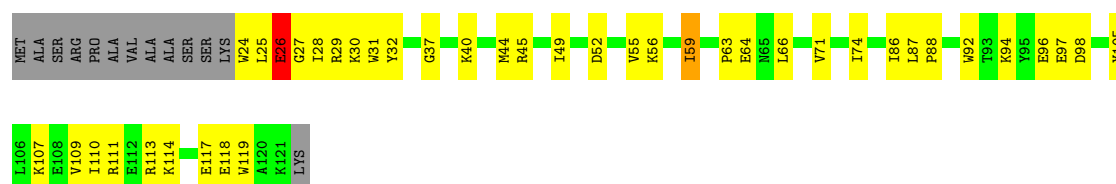
- Molecule 49: Cytochrome b-c1 complex subunit Rieske, mitochondrial





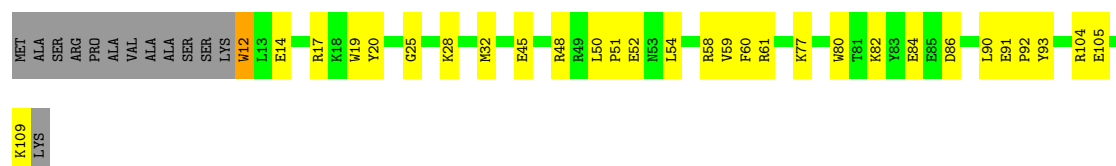
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3F: 51% 35% 12%



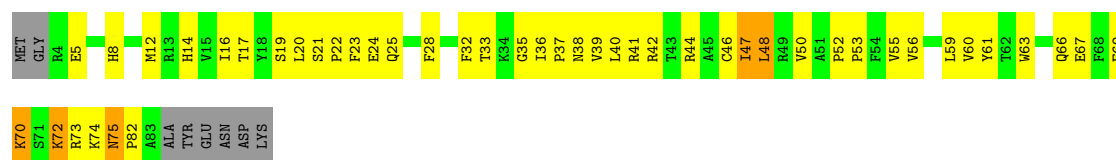
• Molecule 50: Cytochrome b-c1 complex subunit 7

Chain 3S: 61% 26% 12%



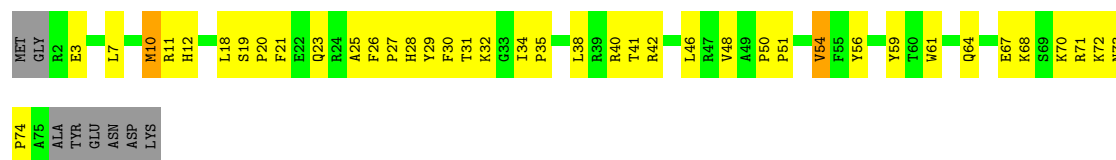
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3G: 34% 50% 6% 10%



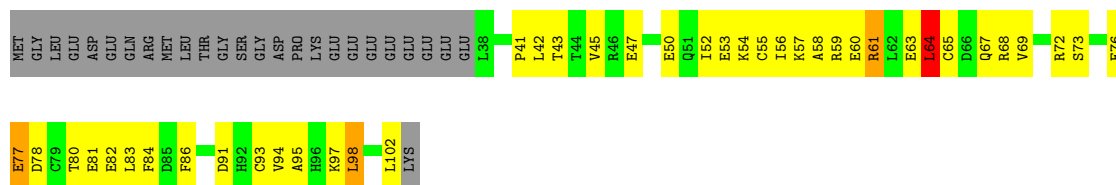
• Molecule 51: Cytochrome b-c1 complex subunit 8

Chain 3T: 41% 46% 10%



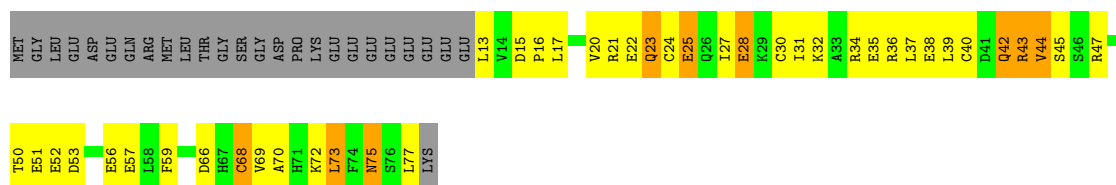
• Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3H: 27% 40% 29%



- Molecule 52: Cytochrome b-c1 complex subunit 6, mitochondrial

Chain 3U: 25% 36% 10% 29%



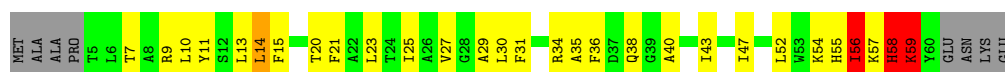
- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3J: 39% 38% 5% 6% 12%



- Molecule 53: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein

Chain 3W: 42% 39% 5% 12%



- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3X: 34% 55% 7%



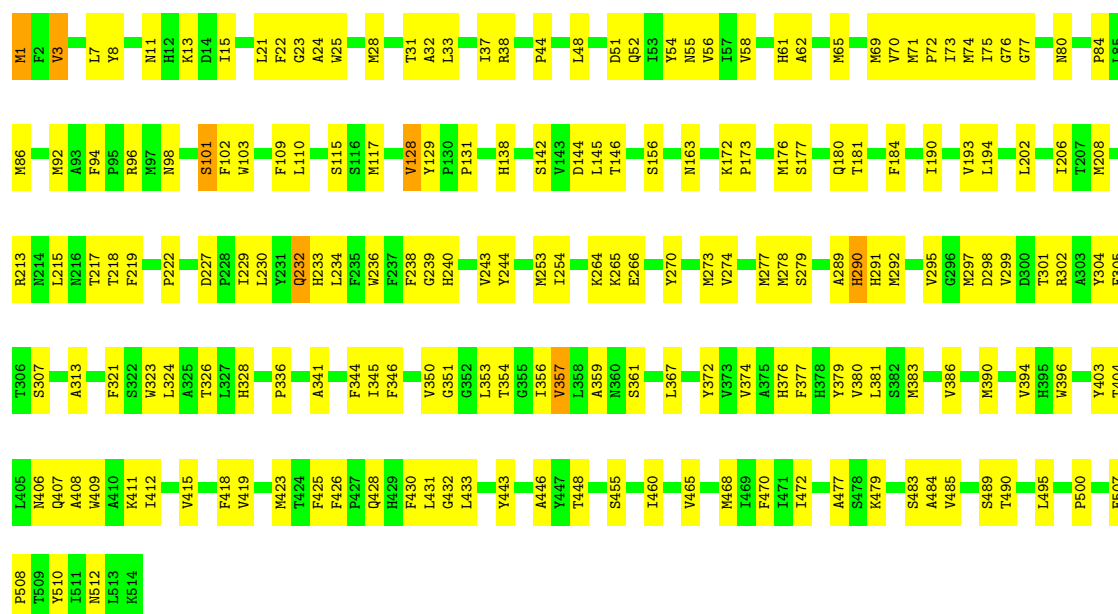
- Molecule 54: Cytochrome b-c1 complex subunit 10

Chain 3Y: 36% 54% 9%



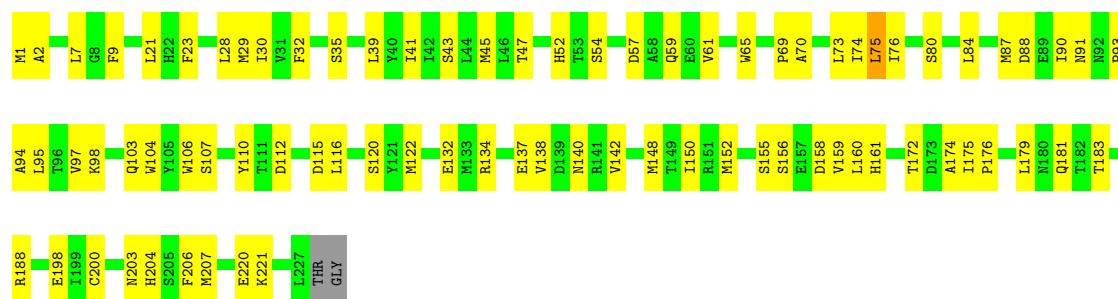
- Molecule 55: Cytochrome c oxidase subunit 1

Chain 4A: 63% 36%



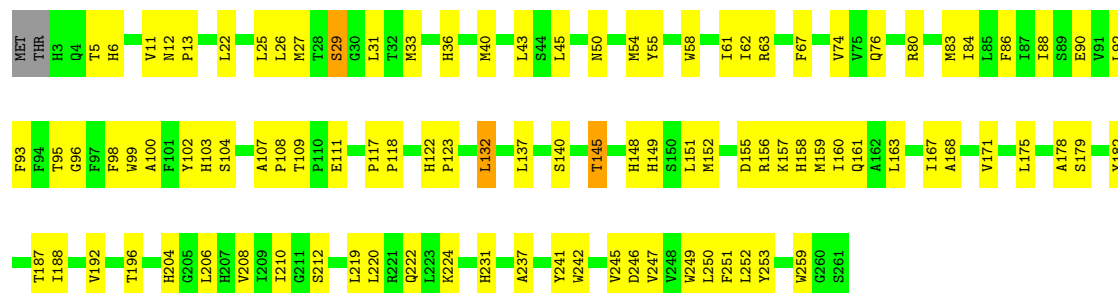
• Molecule 56: Cytochrome c oxidase subunit 2

Chain 4B: 64% 34%



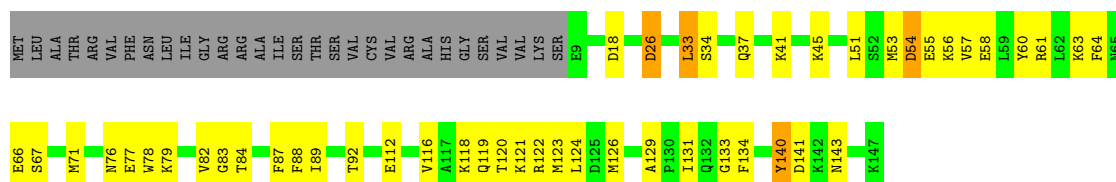
• Molecule 57: Cytochrome c oxidase subunit 3

Chain 4C: 61% 37%



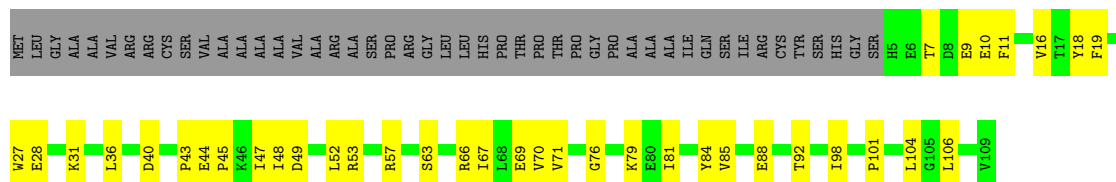
• Molecule 58: Cytochrome c oxidase subunit 4

Chain 4D: 53% 27% 18%



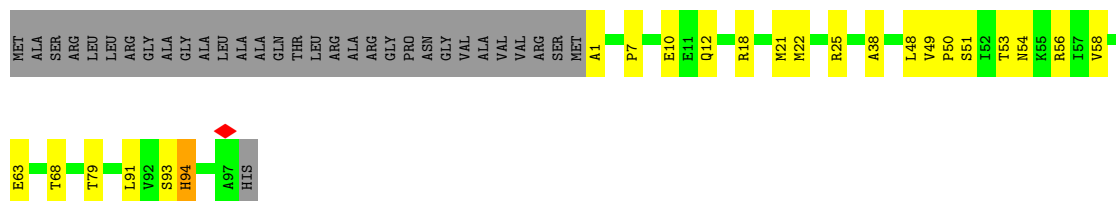
- Molecule 59: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 4E: 44% 25% 31%



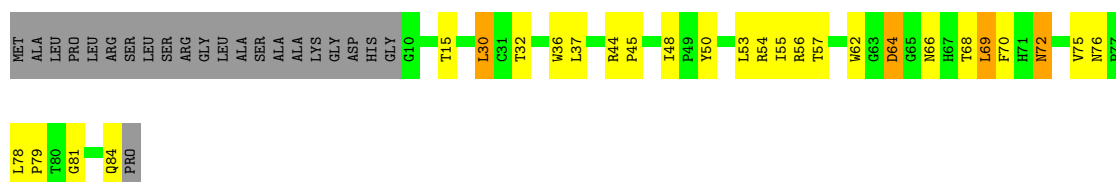
- Molecule 60: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 4F: 57% 17% 25%



- Molecule 61: Cytochrome c oxidase subunit 6A2

Chain 4G: 49% 24% 23%



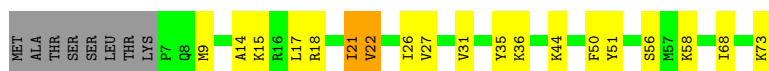
- Molecule 62: Cytochrome c oxidase subunit 6B1

Chain 4H: 56% 37% 5%

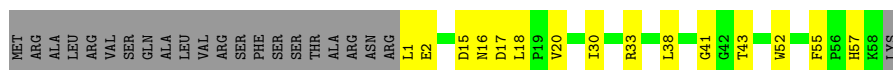


- Molecule 63: Cytochrome c oxidase subunit 6C

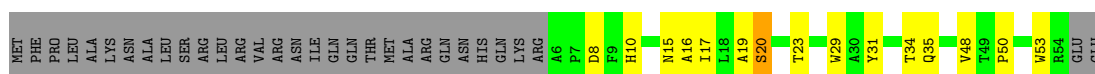
Chain 4I: 64% 23% 11%



- Molecule 64: Cytochrome c oxidase subunit 7A1, mitochondrial



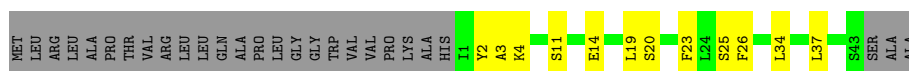
- Molecule 65: Cytochrome c oxidase subunit 7B



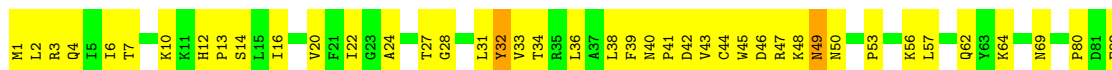
- Molecule 66: Cytochrome c oxidase subunit 7C, mitochondrial



- Molecule 67: Cytochrome c oxidase subunit 8



- Molecule 68: Cytochrome c oxidase subunit NDUF4A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.404	Depositor
Minimum map value	-0.225	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, AME, PO4, ZN, PSC, AYA, CDL, PGT, MG, EHZ, PC1, PGV, 3PE, CU, K, FES, HEA, PEK, CUA, MYR, NDP, NA, GTP, HEM, FME, HEC, SF4, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.42	0/930	0.66	1/1271 (0.1%)
2	1B	0.62	0/1273	0.75	2/1722 (0.1%)
3	1C	0.12	0/1791	0.31	0/2439
4	1D	0.31	0/3545	0.42	2/4806 (0.0%)
5	1E	0.36	0/1698	0.56	2/2311 (0.1%)
6	1F	0.37	0/3401	0.54	11/4595 (0.2%)
7	1G	0.40	0/5451	0.54	9/7387 (0.1%)
8	1H	0.53	0/2566	0.67	9/3509 (0.3%)
9	1I	0.81	0/1443	0.91	9/1952 (0.5%)
10	1J	0.61	0/1364	0.88	7/1850 (0.4%)
11	1K	0.57	1/751 (0.1%)	0.70	4/1018 (0.4%)
12	1L	0.38	0/4939	0.46	5/6718 (0.1%)
13	1M	0.53	0/3713	0.57	3/5063 (0.1%)
14	1N	0.51	0/2765	0.62	5/3758 (0.1%)
15	1O	0.55	3/2650 (0.1%)	0.71	9/3588 (0.3%)
16	1P	0.25	0/2828	0.39	0/3834
17	1Q	0.20	0/1070	0.37	0/1446
18	1R	0.13	0/755	0.32	0/1018
19	1S	0.12	0/711	0.32	0/956
20	1T	0.15	0/701	0.43	0/946
20	1U	0.14	0/706	0.37	0/954
21	1V	0.11	0/946	0.30	0/1281
22	1W	0.12	0/995	0.31	0/1340
23	1X	0.17	0/1436	0.33	0/1938
24	1Y	1.01	0/1037	1.07	7/1404 (0.5%)
25	1Z	0.42	0/1199	0.58	4/1617 (0.2%)
26	1a	0.50	0/577	0.53	0/777
27	1b	0.12	0/664	0.33	0/912
28	1c	0.11	0/430	0.30	0/581
29	1d	0.42	0/1016	0.46	0/1374
30	1e	0.11	0/836	0.31	0/1118

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	1f	0.57	1/499 (0.2%)	0.71	2/673 (0.3%)
32	1g	0.14	0/858	0.37	1/1165 (0.1%)
33	1h	0.12	0/1184	0.31	0/1603
34	1i	0.18	0/1138	0.43	1/1551 (0.1%)
35	1j	0.13	0/627	0.29	0/858
36	1k	0.12	0/668	0.31	0/903
37	1l	0.11	0/1365	0.32	0/1867
38	1m	0.27	0/1092	0.43	0/1481
39	1n	0.15	0/1549	0.35	0/2098
40	1o	0.11	0/1069	0.34	0/1430
41	1p	0.11	0/1481	0.31	0/1997
42	1q	0.56	0/1253	0.59	1/1704 (0.1%)
43	1r	0.45	0/777	0.53	0/1051
44	1s	0.18	0/394	0.45	0/533
45	3A	0.74	0/3481	0.94	14/4722 (0.3%)
45	3N	0.76	0/3496	0.97	15/4723 (0.3%)
46	3B	0.73	0/3190	0.90	7/4317 (0.2%)
46	3O	0.73	0/3175	0.94	8/4292 (0.2%)
47	3C	0.72	0/3123	0.89	10/4269 (0.2%)
47	3P	0.73	0/3122	0.93	12/4269 (0.3%)
48	3D	0.76	0/1946	0.91	2/2641 (0.1%)
48	3Q	0.70	0/1962	0.90	3/2663 (0.1%)
49	3E	0.58	0/1551	0.98	8/2098 (0.4%)
49	3I	0.84	0/342	1.14	2/465 (0.4%)
49	3R	0.63	0/1551	0.95	4/2098 (0.2%)
49	3V	0.67	0/225	0.97	1/303 (0.3%)
50	3F	0.78	0/888	0.99	4/1193 (0.3%)
50	3S	0.70	0/888	0.80	1/1193 (0.1%)
51	3G	0.81	0/648	0.99	2/874 (0.2%)
51	3T	0.69	0/649	0.91	0/878
52	3H	0.79	0/538	0.99	5/721 (0.7%)
52	3U	0.90	0/539	1.09	3/724 (0.4%)
53	3J	1.97	4/476 (0.8%)	3.94	14/641 (2.2%)
53	3W	2.04	3/475 (0.6%)	4.86	9/638 (1.4%)
54	3X	0.67	0/445	0.96	2/608 (0.3%)
54	3Y	0.67	0/437	0.86	0/598
55	4A	0.23	0/4156	0.40	1/5679 (0.0%)
56	4B	0.21	0/1865	0.44	0/2544
57	4C	0.31	0/2179	0.47	1/2981 (0.0%)
58	4D	0.19	0/1197	0.36	0/1617
59	4E	0.20	0/871	0.42	0/1182
60	4F	0.18	0/749	0.42	0/1016
61	4G	0.16	0/644	0.29	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
62	4H	0.26	0/708	0.52	1/956 (0.1%)
63	4I	0.18	0/563	0.34	0/748
64	4J	0.18	0/466	0.30	0/631
65	4K	0.16	0/396	0.34	0/543
66	4L	0.17	0/394	0.34	0/528
67	4M	0.18	0/349	0.29	0/477
68	4N	0.35	0/680	0.60	2/921 (0.2%)
All	All	0.53	12/116505 (0.0%)	0.77	225/158029 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1F	0	1
10	1J	0	1
12	1L	0	1
15	1O	0	1
26	1a	0	1
45	3N	0	2
49	3I	0	2
53	3J	0	3
53	3W	0	3
All	All	0	15

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	3J	59	LYS	C-N	32.71	1.79	1.33
53	3W	56	ILE	C-N	-30.29	0.94	1.33
53	3W	58	HIS	C-N	-22.00	1.02	1.33
53	3J	56	ILE	C-N	-18.58	1.07	1.33
53	3W	59	LYS	C-N	18.10	1.58	1.33
15	1O	175	PRO	CG-CD	-10.88	1.13	1.50
53	3J	57	LYS	C-N	-7.96	1.23	1.32
53	3J	58	HIS	C-N	-7.83	1.22	1.33
15	1O	105	LEU	CA-C	-6.69	1.43	1.52
11	1K	24	SER	CA-C	-6.65	1.44	1.52
15	1O	175	PRO	N-CD	5.98	1.56	1.47
31	1f	34	LEU	N-CA	-5.03	1.41	1.46

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	3W	59	LYS	CA-C-N	-58.59	16.25	121.70
53	3W	59	LYS	C-N-CA	-58.59	16.25	121.70
53	3W	56	ILE	CA-C-N	-55.49	32.31	122.21
53	3W	56	ILE	C-N-CA	-55.49	32.31	122.21
53	3J	57	LYS	O-C-N	-50.33	55.65	122.59
53	3J	58	HIS	O-C-N	-47.63	22.84	121.92
53	3J	56	ILE	CA-C-N	-39.24	46.59	121.54
53	3J	56	ILE	C-N-CA	-39.24	46.59	121.54
53	3J	56	ILE	O-C-N	29.14	152.38	122.07
53	3W	58	HIS	O-C-N	-22.14	93.15	122.59
53	3W	58	HIS	CA-C-N	-20.44	84.91	121.70
53	3W	58	HIS	C-N-CA	-20.44	84.91	121.70
53	3W	59	LYS	O-C-N	16.76	144.89	122.59
53	3J	57	LYS	CA-C-N	-15.75	87.27	121.76
53	3J	57	LYS	C-N-CA	-15.75	87.27	121.76
50	3F	26	GLU	N-CA-C	-14.02	96.00	111.28
15	1O	105	LEU	N-CA-C	-12.63	97.18	111.71
15	1O	175	PRO	CA-N-CD	-11.97	95.24	112.00
15	1O	175	PRO	N-CD-CG	-11.95	85.27	103.20
47	3P	223	TYR	N-CA-C	11.73	125.72	111.40
10	1J	99	MET	N-CA-C	-11.64	97.56	112.23
31	1f	34	LEU	N-CA-C	-10.65	95.84	112.99
8	1H	101	GLY	N-CA-C	10.55	125.70	112.83
25	1Z	139	GLY	N-CA-C	10.32	124.97	112.49
24	1Y	9	SER	N-CA-C	9.76	122.00	111.36
47	3C	223	TYR	N-CA-C	9.74	123.67	111.69
9	1I	28	THR	N-CA-C	9.66	122.82	111.71
52	3U	43	ARG	N-CA-C	-9.49	102.21	113.88
52	3H	64	LEU	N-CA-C	-9.40	101.94	113.41
14	1N	170	LEU	N-CA-C	9.36	122.67	111.82
53	3J	59	LYS	O-C-N	8.89	134.41	122.59
46	3O	153	GLN	N-CA-C	-8.63	102.66	113.01
7	1G	116	LEU	N-CA-C	-8.46	102.00	111.14
8	1H	252	PRO	CA-N-CD	-8.38	100.27	112.00
45	3A	262	TRP	N-CA-C	8.23	119.88	111.07
12	1L	585	LYS	N-CA-C	8.15	120.16	111.28
52	3U	73	LEU	N-CA-C	8.05	120.14	111.36
45	3A	351	GLU	N-CA-C	7.91	119.69	111.14
47	3P	221	HIS	CA-C-N	-7.85	111.07	119.24
47	3P	221	HIS	C-N-CA	-7.85	111.07	119.24
15	1O	131	ASP	N-CA-C	-7.84	103.86	113.50
14	1N	335	LEU	N-CA-C	7.74	122.83	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3E	80	HIS	N-CA-C	-7.70	103.68	113.23
45	3A	232	THR	N-CA-C	-7.64	97.13	109.58
15	1O	303	LYS	N-CA-C	7.63	119.68	111.36
1	1A	27	LEU	N-CA-C	7.61	120.98	109.41
34	1i	117	PRO	CA-N-CD	-7.54	101.44	112.00
9	1I	29	GLU	N-CA-C	-7.45	104.20	113.28
15	1O	82	PHE	N-CA-C	-7.27	103.38	112.90
45	3N	262	TRP	N-CA-C	7.16	119.71	111.11
51	3G	47	ILE	N-CA-C	7.16	117.92	110.62
47	3C	110	LEU	N-CA-C	7.11	118.68	111.07
53	3J	46	HIS	N-CA-C	-7.07	104.28	113.12
7	1G	153	CYS	CA-C-N	-7.05	109.28	121.97
7	1G	153	CYS	C-N-CA	-7.05	109.28	121.97
11	1K	24	SER	CA-C-N	-7.03	112.17	122.65
11	1K	24	SER	C-N-CA	-7.03	112.17	122.65
15	1O	175	PRO	CA-CB-CG	-6.99	91.23	104.50
48	3D	204	ILE	N-CA-C	6.95	117.70	110.62
2	1B	175	ILE	N-CA-C	-6.93	103.72	110.72
46	3O	291	ALA	N-CA-C	6.89	118.79	111.28
45	3N	284	TYR	N-CA-C	6.89	120.12	111.24
47	3P	110	LEU	N-CA-C	6.86	119.34	111.11
6	1F	367	GLU	CA-C-N	6.86	127.59	119.98
6	1F	367	GLU	C-N-CA	6.86	127.59	119.98
47	3C	221	HIS	CA-C-N	-6.84	112.13	119.24
47	3C	221	HIS	C-N-CA	-6.84	112.13	119.24
9	1I	35	GLY	N-CA-C	6.83	120.93	112.73
9	1I	79	ALA	N-CA-C	6.76	120.50	111.30
14	1N	171	ASN	CA-C-N	-6.71	113.46	122.72
14	1N	171	ASN	C-N-CA	-6.71	113.46	122.72
8	1H	252	PRO	N-CD-CG	-6.70	93.15	103.20
24	1Y	6	HIS	N-CA-C	-6.70	104.01	111.71
46	3B	153	GLN	N-CA-C	-6.65	105.14	113.18
47	3P	73	VAL	N-CA-C	-6.60	101.05	109.30
6	1F	189	GLU	N-CA-C	6.60	118.16	110.97
45	3A	314	TYR	N-CA-C	-6.59	100.20	109.69
24	1Y	29	GLY	N-CA-C	-6.50	106.61	114.66
6	1F	407	LEU	N-CA-C	-6.49	104.39	112.90
31	1f	24	CYS	O-C-N	-6.46	114.66	122.22
52	3H	61	ARG	N-CA-C	-6.43	104.36	111.82
47	3P	166	GLY	N-CA-C	-6.39	103.90	114.76
46	3O	32	GLY	N-CA-C	-6.37	106.94	115.21
46	3O	420	GLY	N-CA-C	6.36	120.35	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	3C	256	TYR	N-CA-C	-6.33	105.20	113.17
49	3R	188	ALA	N-CA-C	-6.30	103.94	111.69
6	1F	103	GLY	N-CA-C	-6.24	106.51	114.37
12	1L	585	LYS	N-CA-CB	-6.22	100.97	110.12
24	1Y	115	ALA	N-CA-C	6.21	118.13	111.36
7	1G	203	CYS	CA-C-N	-6.21	113.33	120.04
7	1G	203	CYS	C-N-CA	-6.21	113.33	120.04
48	3Q	155	GLY	N-CA-C	-6.20	107.32	114.69
45	3N	30	SER	N-CA-C	-6.17	100.26	108.34
45	3N	238	GLY	N-CA-C	-6.14	101.38	110.97
45	3N	226	ASP	N-CA-C	-6.13	104.29	112.94
2	1B	132	VAL	N-CA-C	6.09	116.70	108.17
42	1q	26	VAL	N-CA-C	6.01	118.61	111.09
45	3N	411	CYS	N-CA-C	-6.01	104.85	111.82
46	3B	170	ASN	N-CA-C	6.00	123.58	110.80
12	1L	560	THR	N-CA-C	6.00	117.48	111.07
53	3J	59	LYS	CA-C-N	-5.99	110.91	121.70
53	3J	59	LYS	C-N-CA	-5.99	110.91	121.70
45	3A	238	GLY	N-CA-C	-5.98	101.65	110.97
47	3C	28	SER	N-CA-C	5.96	119.10	109.86
68	4N	32	TYR	N-CA-C	-5.96	102.80	110.19
13	1M	89	THR	N-CA-C	5.94	117.75	111.28
9	1I	133	GLU	N-CA-C	-5.94	99.56	109.24
46	3O	203	ARG	N-CA-C	-5.91	103.75	113.50
8	1H	252	PRO	CA-CB-CG	-5.91	93.27	104.50
47	3C	241	ILE	N-CA-C	-5.89	104.77	110.72
46	3O	328	SER	N-CA-C	5.89	117.10	108.14
50	3S	25	GLY	N-CA-C	5.89	123.78	115.30
8	1H	76	ILE	N-CA-C	5.85	116.62	110.72
53	3J	53	TRP	N-CA-C	-5.85	100.30	109.25
52	3H	98	LEU	N-CA-C	5.83	117.71	111.36
5	1E	101	GLN	CA-C-N	-5.80	116.00	123.19
5	1E	101	GLN	C-N-CA	-5.80	116.00	123.19
12	1L	583	LEU	O-C-N	-5.79	116.55	123.27
46	3B	234	GLY	N-CA-C	5.79	118.70	112.33
49	3I	42	VAL	N-CA-C	-5.78	103.68	110.21
47	3C	166	GLY	N-CA-C	-5.77	104.01	114.46
24	1Y	28	GLY	N-CA-C	5.77	119.47	112.49
46	3O	347	ILE	N-CA-C	-5.76	104.90	110.72
10	1J	16	GLY	O-C-N	-5.75	116.02	122.28
49	3I	70	LEU	N-CA-C	-5.75	100.87	109.15
54	3X	4	ARG	N-CA-C	-5.74	105.17	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	4H	23	GLN	N-CA-C	5.74	118.40	111.40
12	1L	586	LEU	N-CA-C	-5.73	105.01	112.23
6	1F	101	GLU	CA-C-N	-5.73	113.86	119.76
6	1F	101	GLU	C-N-CA	-5.73	113.86	119.76
46	3B	201	SER	N-CA-C	5.72	117.52	111.28
54	3X	7	GLY	N-CA-C	5.70	123.96	112.34
45	3A	286	GLY	N-CA-C	5.69	124.54	115.66
47	3C	184	ILE	N-CA-C	5.67	116.45	110.72
9	1I	37	THR	N-CA-C	-5.65	104.74	111.69
6	1F	408	GLY	N-CA-C	-5.65	105.95	112.50
24	1Y	46	ALA	N-CA-C	-5.61	106.48	113.38
48	3D	199	PRO	N-CA-C	5.60	120.28	111.38
25	1Z	138	TYR	CA-C-N	5.59	126.03	119.94
25	1Z	138	TYR	C-N-CA	5.59	126.03	119.94
7	1G	151	THR	N-CA-C	-5.59	106.46	113.28
45	3N	277	ILE	N-CA-C	-5.58	104.92	111.00
45	3N	416	TYR	N-CA-C	5.58	117.78	109.59
46	3B	73	SER	N-CA-C	-5.57	102.78	110.35
45	3A	203	VAL	N-CA-C	5.57	115.88	107.75
50	3F	64	GLU	N-CA-C	5.53	116.99	111.07
45	3N	208	LEU	N-CA-C	-5.52	105.34	111.36
4	1D	342	MET	N-CA-C	5.52	116.98	111.07
9	1I	117	ILE	N-CA-C	-5.52	107.90	113.47
10	1J	65	LEU	CA-C-N	5.51	131.88	121.97
10	1J	65	LEU	C-N-CA	5.51	131.88	121.97
9	1I	26	LEU	N-CA-C	-5.50	105.79	112.88
7	1G	182	GLN	CA-C-N	-5.49	115.98	123.12
7	1G	182	GLN	C-N-CA	-5.49	115.98	123.12
49	3E	269	ASP	N-CA-C	-5.47	104.10	111.54
57	4C	250	LEU	N-CA-C	-5.47	105.42	111.71
55	4A	232	GLN	N-CA-C	-5.46	105.43	111.71
8	1H	101	GLY	CA-C-O	-5.46	115.45	120.80
49	3R	266	THR	N-CA-C	-5.45	105.93	113.18
15	1O	125	GLU	N-CA-C	-5.45	98.08	108.17
15	1O	175	PRO	N-CA-CB	-5.45	98.74	103.32
53	3J	58	HIS	CB-CA-C	-5.45	109.31	115.79
8	1H	252	PRO	CB-CG-CD	-5.43	88.73	106.10
6	1F	184	TYR	N-CA-C	5.43	118.11	111.82
4	1D	426	GLY	N-CA-C	-5.41	108.24	115.32
45	3N	27	SER	N-CA-C	5.40	117.98	108.75
6	1F	104	THR	N-CA-C	5.38	117.52	108.96
45	3A	428	ILE	N-CA-C	5.38	117.37	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	3J	54	LYS	N-CA-C	-5.38	99.34	110.80
11	1K	24	SER	N-CA-C	-5.38	107.08	113.97
48	3Q	44	ASP	N-CA-C	5.38	118.63	111.75
45	3A	411	CYS	N-CA-C	-5.37	105.59	111.82
13	1M	5	ILE	N-CA-C	5.37	116.14	110.72
47	3P	28	SER	N-CA-C	5.36	118.17	109.86
8	1H	100	LEU	N-CA-C	5.36	116.87	110.44
49	3R	150	SER	N-CA-C	-5.34	105.40	112.34
52	3H	76	GLU	N-CA-C	-5.34	105.50	112.23
14	1N	153	LEU	N-CA-C	-5.34	105.13	111.69
25	1Z	36	PHE	N-CA-C	-5.32	106.29	112.89
52	3U	44	VAL	N-CA-C	-5.27	105.40	110.72
8	1H	99	ASN	N-CA-C	-5.26	106.37	112.89
48	3Q	25	SER	N-CA-C	-5.26	105.60	112.23
45	3A	368	HIS	CA-C-O	-5.26	115.28	120.80
47	3P	241	ILE	N-CA-C	-5.26	105.37	110.42
47	3P	362	ILE	N-CA-C	5.24	115.97	110.62
6	1F	361	GLN	N-CA-C	5.24	116.67	111.07
50	3F	37	GLY	N-CA-C	5.23	122.84	115.30
49	3V	49	PHE	N-CA-C	-5.23	99.89	108.41
13	1M	3	LYS	N-CA-C	-5.22	106.74	113.01
49	3R	82	ASP	N-CA-C	-5.22	106.59	113.17
49	3E	244	ASP	N-CA-C	5.21	115.42	108.38
47	3P	145	VAL	N-CA-C	5.21	115.43	110.53
46	3B	144	LEU	N-CA-C	-5.21	105.50	111.07
49	3E	200	HIS	N-CA-C	5.19	117.23	110.43
53	3W	14	LEU	N-CA-C	5.18	119.75	113.38
45	3N	348	SER	N-CA-C	5.17	117.45	110.06
46	3O	248	ASN	N-CA-C	-5.16	106.53	114.16
49	3E	223	VAL	N-CA-C	5.16	120.02	108.88
68	4N	31	LEU	N-CA-C	-5.16	105.66	111.28
10	1J	35	VAL	N-CA-C	-5.15	105.37	110.62
52	3H	77	GLU	N-CA-C	-5.14	102.07	110.20
45	3A	422	VAL	N-CA-C	5.14	116.12	108.46
47	3P	86	GLY	N-CA-C	-5.12	107.96	114.16
10	1J	34	ILE	N-CA-C	5.09	115.82	110.62
7	1G	117	GLN	N-CA-C	5.09	116.64	111.14
32	1g	30	PRO	CA-N-CD	-5.09	104.88	112.00
47	3C	206	ASN	N-CA-C	-5.08	103.98	110.53
24	1Y	35	VAL	N-CA-C	-5.08	105.59	110.72
46	3B	94	GLY	N-CA-C	5.07	121.02	112.85
50	3F	59	ILE	N-CA-C	5.07	115.84	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	3E	210	TRP	N-CA-C	5.07	115.81	107.20
49	3E	232	GLY	N-CA-C	-5.07	108.62	115.21
9	1I	71	PRO	CA-N-CD	-5.07	104.91	112.00
45	3A	27	SER	N-CA-C	5.04	117.56	108.48
47	3P	347	PHE	N-CA-C	5.04	117.67	111.82
45	3N	281	ASP	N-CA-C	-5.04	101.42	109.23
49	3E	183	GLU	N-CA-C	-5.04	105.49	111.69
45	3N	194	ARG	N-CA-C	-5.04	107.17	113.72
45	3A	232	THR	CA-C-N	-5.03	114.53	119.92
45	3A	232	THR	C-N-CA	-5.03	114.53	119.92
51	3G	70	LYS	N-CA-C	-5.02	106.84	113.17
10	1J	21	SER	N-CA-C	-5.01	106.68	112.89
45	3N	278	GLY	N-CA-C	5.01	120.08	111.47
11	1K	22	TYR	N-CA-C	5.00	117.31	110.55
45	3N	173	ASN	N-CA-C	-5.00	105.93	112.23

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
10	1J	86	ASN	Mainchain
12	1L	583	LEU	Mainchain
15	1O	301	GLY	Mainchain
26	1a	37	ARG	Mainchain
49	3I	47	ARG	Sidechain
49	3I	52	ARG	Sidechain
53	3J	56	ILE	Mainchain
53	3J	57	LYS	Mainchain
53	3J	58	HIS	Mainchain
45	3N	206	ARG	Mainchain
53	3W	56	ILE	Mainchain
53	3W	58	HIS	Mainchain
53	3W	59	LYS	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	103	0
2	1B	1242	0	1250	123	0
3	1C	1740	0	1691	30	0
4	1D	3452	0	3389	123	0
5	1E	1658	0	1664	75	0
6	1F	3325	0	3290	138	0
7	1G	5362	0	5391	174	0
8	1H	2504	0	2602	169	0
9	1I	1412	0	1368	71	0
10	1J	1329	0	1326	131	0
11	1K	750	0	798	62	0
12	1L	4818	0	4956	275	0
13	1M	3632	0	3836	184	0
14	1N	2712	0	2873	171	0
15	1O	2590	0	2556	114	0
16	1P	2751	0	2776	96	0
17	1Q	1047	0	1042	37	0
18	1R	741	0	704	13	0
19	1S	700	0	719	18	0
20	1T	689	0	687	30	0
20	1U	694	0	691	30	0
21	1V	927	0	972	20	0
22	1W	971	0	975	22	0
23	1X	1398	0	1378	34	0
24	1Y	1016	0	1012	232	0
25	1Z	1168	0	1161	47	0
26	1a	562	0	557	30	0
27	1b	643	0	645	44	0
28	1c	417	0	425	20	0
29	1d	985	0	978	67	0
30	1e	816	0	823	18	0
31	1f	487	0	493	74	0
32	1g	835	0	793	55	0
33	1h	1151	0	1164	87	0
34	1i	1100	0	1107	57	0
35	1j	601	0	546	27	0
36	1k	649	0	626	6	0
37	1l	1310	0	1204	41	0
38	1m	1062	0	1075	95	0
39	1n	1495	0	1431	54	0
40	1o	1045	0	1016	58	0
41	1p	1449	0	1416	42	0
42	1q	1212	0	1174	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	1r	759	0	783	29	0
44	1s	382	0	351	15	0
45	3A	3411	0	3309	138	0
45	3N	3424	0	3350	166	0
46	3B	3138	0	3116	143	0
46	3O	3124	0	3108	139	0
47	3C	3025	0	3090	236	0
47	3P	3024	0	3090	214	0
48	3D	1888	0	1834	110	0
48	3Q	1904	0	1849	131	0
49	3E	1518	0	1499	220	0
49	3I	337	0	347	41	0
49	3R	1518	0	1499	253	0
49	3V	223	0	233	21	0
50	3F	868	0	857	42	0
50	3S	868	0	857	30	0
51	3G	628	0	634	68	0
51	3T	628	0	634	63	0
52	3H	533	0	512	37	0
52	3U	533	0	513	46	0
53	3J	464	0	464	63	0
53	3W	464	0	462	37	0
54	3X	429	0	430	72	0
54	3Y	421	0	418	86	0
55	4A	4026	0	4005	203	0
56	4B	1828	0	1836	80	0
57	4C	2096	0	2027	109	0
58	4D	1163	0	1143	42	0
59	4E	852	0	845	27	0
60	4F	734	0	718	20	0
61	4G	617	0	585	34	0
62	4H	687	0	645	26	0
63	4I	550	0	560	26	0
64	4J	456	0	456	23	0
65	4K	383	0	366	16	0
66	4L	381	0	380	38	0
67	4M	338	0	345	11	0
68	4N	660	0	664	47	0
69	1A	88	0	127	33	0
69	1B	102	0	163	44	0
69	1J	95	0	144	51	0
69	1L	473	0	679	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
69	1M	47	0	71	13	0
69	1N	51	0	82	57	0
69	1Y	539	0	803	257	0
69	1Z	51	0	82	12	0
69	1b	42	0	61	31	0
69	1d	146	0	215	104	0
69	1e	51	0	82	15	0
69	1f	181	0	253	124	0
69	1g	84	0	122	43	0
69	1h	47	0	71	15	0
69	1k	46	0	67	32	0
69	1l	126	0	180	27	0
69	1m	236	0	357	91	0
69	1o	51	0	82	31	0
69	3A	102	0	164	61	0
69	3C	691	0	1046	267	0
69	3D	86	0	123	19	0
69	3E	100	0	157	27	0
69	3G	424	0	577	113	0
69	3J	238	0	363	63	0
69	3N	102	0	164	65	0
69	3P	772	0	1202	281	0
69	3Q	133	0	194	39	0
69	3R	153	0	246	59	0
69	3S	51	0	82	26	0
69	3T	51	0	82	26	0
69	3W	144	0	225	67	0
69	3X	255	0	410	121	0
69	3Y	281	0	433	109	0
69	4G	73	0	94	34	0
70	1A	35	0	44	28	0
70	1B	94	0	134	88	0
70	1H	143	0	220	58	0
70	1J	35	0	44	7	0
70	1M	44	0	65	12	0
70	1P	33	0	40	6	0
70	1Y	135	0	192	82	0
70	1d	39	0	52	24	0
70	1h	93	0	140	29	0
70	3J	54	0	88	13	0
70	3P	54	0	88	15	0
70	3R	54	0	88	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	3T	54	0	88	45	0
70	3X	54	0	88	17	0
71	1B	8	0	0	1	0
71	1F	8	0	0	8	0
71	1G	16	0	0	4	0
71	1I	16	0	0	3	0
72	1E	4	0	0	4	0
72	1G	4	0	0	4	0
72	3E	4	0	0	5	0
72	3R	4	0	0	4	0
73	1F	31	0	19	4	0
74	1G	1	0	0	0	0
75	1H	51	0	46	10	0
75	1L	87	0	124	38	0
75	1N	77	0	98	33	0
75	1Y	100	0	156	39	0
75	1d	179	0	264	60	0
75	1g	100	0	154	60	0
75	1i	80	0	104	35	0
75	1q	161	0	221	40	0
75	3A	98	0	149	45	0
75	3D	56	0	56	4	0
75	3F	100	0	156	26	0
75	3N	100	0	156	57	0
75	3P	100	0	156	60	0
75	3T	57	0	58	13	0
75	3X	100	0	156	31	0
75	3Y	100	0	156	31	0
75	4B	100	0	156	40	0
75	4C	200	0	312	41	0
76	1I	8	0	8	6	0
77	1O	32	0	12	7	0
78	1O	1	0	0	0	0
78	4A	1	0	0	0	0
79	1P	48	0	26	2	0
80	1R	1	0	0	0	0
80	4F	1	0	0	0	0
81	1T	37	0	0	0	0
81	1n	37	0	0	1	0
82	1Y	51	0	78	24	0
83	1h	11	0	12	2	0
84	1l	15	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	3C	86	0	60	8	0
85	3P	86	0	60	5	0
86	3D	42	0	32	6	0
86	3Q	43	0	32	10	0
87	3X	53	0	77	9	0
87	4G	52	0	72	13	0
88	4A	120	0	108	11	0
89	4A	1	0	0	0	0
90	4A	1	0	0	0	0
91	4A	204	0	304	104	0
91	4C	255	0	376	66	0
91	4G	51	0	76	10	0
91	4J	42	0	57	8	0
91	4K	43	0	59	7	0
91	4N	51	0	76	13	0
92	4B	2	0	0	0	0
93	4B	52	0	80	27	0
94	4H	5	0	0	0	0
All	All	124052	0	128247	7317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (7317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3P:514:3PE:H121	54:3Y:2:LEU:CD1	1.30	1.61
69:1d:201:3PE:C2G	69:1d:201:3PE:C3C	1.74	1.60
37:1l:111:PHE:CD2	69:1l:203:3PE:H281	1.35	1.59
69:1d:201:3PE:C2G	69:1d:201:3PE:C3D	1.80	1.58
47:3P:306:MET:HE2	69:3P:514:3PE:C25	1.13	1.57
47:3P:306:MET:CE	69:3P:514:3PE:C26	1.85	1.55
91:4A:609:PGV:C19	66:4L:28:TYR:CE1	1.89	1.54
69:3P:503:3PE:C1	69:3P:503:3PE:H241	1.34	1.54
2:1B:176:TRP:CZ2	70:1B:202:PC1:C23	1.94	1.51
2:1B:176:TRP:CH2	70:1B:202:PC1:C23	1.93	1.50
61:4G:37:LEU:CD2	69:4G:104:3PE:N	1.73	1.50
35:1j:38:TRP:CH2	69:1k:101:3PE:H341	1.47	1.48
35:1j:38:TRP:CZ2	69:1k:101:3PE:H371	1.50	1.47
24:1Y:5:LEU:CD1	69:1Y:211:3PE:H331	1.44	1.45
47:3P:306:MET:CE	69:3P:514:3PE:H261	1.43	1.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:306:MET:CE	69:3P:514:3PE:C25	1.92	1.43
10:1J:99:MET:CE	69:1J:201:3PE:H3I2	1.49	1.43
24:1Y:62:SER:CB	69:1Y:208:3PE:H371	1.49	1.43
53:3J:57:LYS:CG	53:3J:58:HIS:H	1.12	1.42
24:1Y:5:LEU:HD11	69:1Y:211:3PE:C33	1.49	1.40
31:1f:28:ARG:HH22	69:1f:103:3PE:C3	1.31	1.40
69:3P:503:3PE:H12	69:3P:503:3PE:C24	1.50	1.40
69:1d:201:3PE:C2G	69:1d:201:3PE:H3D1	1.40	1.40
28:1c:30:TYR:CE2	69:1d:203:3PE:H341	1.55	1.39
47:3P:306:MET:HE1	69:3P:514:3PE:C26	1.41	1.39
10:1J:99:MET:HE2	69:1J:201:3PE:C3I	1.50	1.39
31:1f:28:ARG:NH2	69:1f:103:3PE:H31	1.07	1.39
69:3P:508:3PE:C3I	75:3P:513:CDL:H441	1.52	1.39
53:3J:59:LYS:C	53:3J:60:TYR:N	1.79	1.38
10:1J:99:MET:SD	69:1J:203:3PE:H3C1	1.61	1.38
47:3C:284:ILE:CD1	69:3C:512:3PE:H352	1.55	1.37
69:3C:510:3PE:H12	69:3C:510:3PE:C12	1.54	1.36
55:4A:1:FME:CN	91:4A:609:PGV:O05	1.72	1.35
69:1L:710:3PE:H221	33:1h:26:ARG:NH1	1.37	1.35
69:1B:205:3PE:H342	69:1B:205:3PE:C3	1.58	1.33
24:1Y:62:SER:HB3	69:1Y:208:3PE:C37	1.58	1.32
91:4A:609:PGV:O04	66:4L:28:TYR:CE1	1.79	1.31
2:1B:176:TRP:CE2	70:1B:202:PC1:C23	2.12	1.31
53:3J:17:ARG:CD	69:3J:103:3PE:H2	1.61	1.31
35:1j:38:TRP:NE1	69:1k:101:3PE:H382	1.44	1.30
53:3J:17:ARG:HD3	69:3J:103:3PE:C2	1.60	1.29
69:3P:514:3PE:C12	54:3Y:2:LEU:CD1	2.10	1.29
69:3P:514:3PE:C12	54:3Y:2:LEU:HD13	1.59	1.29
47:3P:306:MET:CE	69:3P:514:3PE:H252	1.57	1.29
2:1B:176:TRP:CZ3	70:1B:202:PC1:C23	2.16	1.29
1:1A:23:TRP:CE2	70:1A:202:PC1:O12	1.86	1.28
69:1d:201:3PE:H2H1	69:1d:201:3PE:C3F	1.62	1.28
1:1A:22:PHE:HD2	70:1A:202:PC1:O32	1.13	1.27
70:1B:202:PC1:H241	70:1B:202:PC1:C2A	1.64	1.27
12:1L:567:SER:OG	69:1L:705:3PE:H322	1.29	1.27
31:1f:10:HIS:ND1	69:1f:102:3PE:H232	1.50	1.27
56:4B:7:LEU:CD1	75:4B:302:CDL:H712	1.65	1.25
2:1B:177:TYR:HA	70:1B:202:PC1:C25	1.66	1.25
69:1L:710:3PE:C22	33:1h:26:ARG:HH11	1.49	1.25
35:1j:38:TRP:CE2	69:1k:101:3PE:H371	1.71	1.25
24:1Y:108:GLY:CA	70:1Y:206:PC1:H232	1.66	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:34:GLN:NE2	69:1d:203:3PE:H121	1.52	1.24
91:4A:609:PGV:C19	66:4L:28:TYR:CZ	2.20	1.24
2:1B:176:TRP:CE2	70:1B:202:PC1:C24	2.20	1.23
54:3Y:4:ARG:NH2	69:3Y:107:3PE:O11	1.71	1.23
69:1d:206:3PE:H381	69:1f:104:3PE:C2B	1.67	1.23
1:1A:22:PHE:CD2	70:1A:202:PC1:O32	1.91	1.23
48:3Q:37:CYS:SG	86:3Q:501:HEC:HBB3	1.79	1.23
54:3X:44:TRP:CH2	69:3X:108:3PE:H372	1.73	1.22
69:1B:205:3PE:C3	69:1B:205:3PE:C34	2.17	1.22
47:3C:284:ILE:HD12	69:3C:512:3PE:C35	1.70	1.22
48:3Q:40:CYS:SG	86:3Q:501:HEC:CAC	2.28	1.22
47:3C:352:GLN:NE2	69:3C:511:3PE:H221	1.53	1.21
27:1b:27:LEU:CD1	69:1b:101:3PE:H2D1	1.69	1.21
38:1m:92:PHE:CD1	69:1m:203:3PE:H271	1.75	1.21
38:1m:99:PHE:CE2	69:1m:205:3PE:H3G2	1.77	1.20
12:1L:517:SER:OG	69:1L:708:3PE:H11	1.41	1.20
10:1J:99:MET:CE	69:1J:201:3PE:H3F1	1.71	1.20
47:3P:306:MET:HE2	69:3P:514:3PE:C24	1.71	1.20
51:3G:44:ARG:HH22	69:3G:105:3PE:C12	1.55	1.19
69:1d:201:3PE:C2F	69:1d:201:3PE:C3B	2.20	1.19
61:4G:37:LEU:CD2	69:4G:104:3PE:HN3	1.41	1.19
10:1J:99:MET:SD	69:1J:203:3PE:C3C	2.29	1.19
69:3C:510:3PE:H122	69:3C:510:3PE:C1	1.71	1.19
24:1Y:62:SER:OG	69:1Y:208:3PE:H341	1.39	1.18
69:1B:205:3PE:C34	69:1B:205:3PE:H32	1.74	1.18
24:1Y:5:LEU:HD21	69:1Y:211:3PE:C32	1.73	1.18
24:1Y:75:ILE:HG23	69:1Y:201:3PE:H271	1.25	1.18
91:4C:302:PGV:C29	75:4C:307:CDL:H402	1.73	1.18
24:1Y:5:LEU:HD21	69:1Y:211:3PE:H321	1.24	1.17
27:1b:27:LEU:HD12	69:1b:101:3PE:C2D	1.73	1.17
70:1B:202:PC1:H241	70:1B:202:PC1:C29	1.73	1.17
31:1f:22:PHE:HB2	69:1f:104:3PE:H3B2	1.21	1.17
2:1B:176:TRP:CZ2	70:1B:202:PC1:C24	2.26	1.17
69:1d:206:3PE:C37	69:1f:104:3PE:H2B1	1.74	1.17
38:1m:24:ILE:O	45:3N:227:ALA:CB	1.94	1.16
37:1l:111:PHE:CD2	69:1l:203:3PE:C28	2.28	1.16
47:3P:306:MET:HE1	69:3P:514:3PE:C27	1.75	1.16
69:3P:514:3PE:H121	54:3Y:2:LEU:HD11	1.22	1.16
93:4B:303:PSC:H072	63:4I:14:ALA:HB2	1.26	1.16
69:1d:206:3PE:C38	69:1f:104:3PE:H2B1	1.73	1.15
69:1L:703:3PE:H2	40:1o:77:LEU:CD1	1.77	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:77:LEU:HB2	69:1o:201:3PE:H261	1.30	1.14
69:3P:511:3PE:H2A1	69:3P:511:3PE:H2E1	1.26	1.14
27:1b:27:LEU:HD11	69:1b:101:3PE:H2F2	1.28	1.14
69:1L:703:3PE:C2	40:1o:77:LEU:HD11	1.76	1.13
61:4G:37:LEU:HD23	69:4G:104:3PE:C12	1.76	1.13
38:1m:92:PHE:CE2	69:1m:203:3PE:H231	1.83	1.13
75:3A:501:CDL:O1	69:3A:503:3PE:H12	1.44	1.13
53:3J:17:ARG:HD2	69:3J:103:3PE:O11	1.48	1.13
6:1F:405:CYS:SG	71:1F:502:SF4:FE2	1.39	1.13
47:3P:10:LEU:HD23	69:3P:512:3PE:H381	1.25	1.12
24:1Y:108:GLY:HA2	70:1Y:206:PC1:H232	1.13	1.12
69:1d:201:3PE:C3D	69:1d:201:3PE:C2F	2.09	1.12
49:3R:235:TYR:HA	49:3R:242:HIS:HA	1.26	1.12
91:4C:302:PGV:H292	75:4C:307:CDL:H402	1.25	1.12
24:1Y:27:ILE:HB	69:1Y:208:3PE:H3D2	1.29	1.12
49:3R:217:CYS:HB2	49:3R:224:PRO:HD3	1.30	1.12
13:1M:22:MET:HE1	69:1g:202:3PE:H221	1.30	1.12
47:3P:10:LEU:HD23	69:3P:512:3PE:C38	1.79	1.12
24:1Y:75:ILE:CG2	69:1Y:201:3PE:H271	1.79	1.11
48:3Q:37:CYS:SG	86:3Q:501:HEC:CBB	2.36	1.11
47:3P:306:MET:HE2	69:3P:514:3PE:C26	1.61	1.11
8:1H:99:ASN:OD1	70:1H:403:PC1:H151	1.48	1.11
38:1m:87:LEU:HD12	69:1m:202:3PE:H251	1.25	1.11
38:1m:92:PHE:HE1	69:1m:203:3PE:C37	1.62	1.10
49:3E:241:SER:HA	49:3E:252:GLY:HA3	1.12	1.10
51:3G:56:VAL:HG21	69:3G:109:3PE:H2A2	1.22	1.10
10:1J:99:MET:SD	69:1J:203:3PE:C3D	2.39	1.10
31:1f:21:VAL:HG23	69:1f:104:3PE:C3E	1.81	1.10
28:1c:30:TYR:HE2	69:1d:203:3PE:C34	1.65	1.10
29:1d:8:ARG:HD3	70:1d:204:PC1:C23	1.81	1.10
2:1B:42:ARG:NH1	70:1B:203:PC1:O12	1.85	1.10
2:1B:176:TRP:CD2	70:1B:202:PC1:C24	2.34	1.10
35:1j:38:TRP:CE2	69:1k:101:3PE:C37	2.34	1.10
24:1Y:75:ILE:HG22	69:1Y:214:3PE:H261	1.29	1.09
35:1j:38:TRP:CZ2	69:1k:101:3PE:C37	2.35	1.09
54:3Y:41:ILE:HD13	69:3Y:105:3PE:H371	1.31	1.09
75:4B:302:CDL:OA9	63:4I:35:TYR:CD1	2.03	1.09
24:1Y:87:LEU:HD13	69:1Y:212:3PE:H332	1.26	1.09
47:3P:92:ILE:HD11	69:3P:519:3PE:H291	1.27	1.09
47:3P:249:LEU:CD1	69:3P:520:3PE:H2	1.82	1.09
61:4G:37:LEU:HD23	69:4G:104:3PE:N	1.50	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:176:TRP:CD2	70:1B:202:PC1:C23	2.34	1.09
51:3G:44:ARG:HH12	69:3G:107:3PE:H112	1.16	1.09
10:1J:99:MET:HE1	69:1J:201:3PE:H3F1	1.18	1.09
69:1L:710:3PE:C22	33:1h:26:ARG:NH1	2.08	1.09
37:1l:111:PHE:CE2	69:1l:203:3PE:H281	1.88	1.09
55:4A:406:ASN:OD1	91:4A:606:PGV:O14	1.69	1.09
75:1L:704:CDL:H142	13:1M:361:MET:HE1	1.11	1.08
24:1Y:122:ALA:HB1	70:1Y:202:PC1:H351	1.34	1.08
75:3A:501:CDL:C52	69:3A:503:3PE:H272	1.83	1.08
54:3X:44:TRP:CZ2	69:3X:108:3PE:H221	1.89	1.08
12:1L:602:PHE:CE2	69:1L:706:3PE:O32	2.06	1.08
2:1B:176:TRP:CE3	70:1B:202:PC1:C23	2.36	1.08
14:1N:301:SER:O	69:1N:401:3PE:H342	1.53	1.08
55:4A:1:FME:HCN	91:4A:609:PGV:O05	1.50	1.08
2:1B:176:TRP:O	70:1B:202:PC1:H252	1.53	1.07
70:1B:202:PC1:H221	16:1P:275:PHE:HE1	1.13	1.07
2:1B:176:TRP:CH2	70:1B:202:PC1:H232	1.78	1.07
8:1H:77:LEU:HD12	70:1H:403:PC1:C3C	1.82	1.07
8:1H:99:ASN:OD1	70:1H:403:PC1:C15	2.02	1.07
24:1Y:80:ARG:HG2	69:1Y:214:3PE:O14	1.52	1.07
61:4G:37:LEU:HD21	69:4G:104:3PE:HN3	1.12	1.07
75:1g:201:CDL:H391	33:1h:32:THR:HG22	1.27	1.07
38:1m:92:PHE:CE1	69:1m:203:3PE:H371	1.88	1.07
55:4A:109:PHE:HB3	91:4A:609:PGV:H171	1.12	1.07
32:1g:68:ILE:HD13	75:1g:201:CDL:H261	1.30	1.07
53:3J:17:ARG:HD3	69:3J:103:3PE:H2	1.12	1.07
69:1d:201:3PE:C3F	69:1d:201:3PE:C2H	2.31	1.07
31:1f:21:VAL:HG23	69:1f:104:3PE:H3E1	1.31	1.07
54:3X:44:TRP:CZ3	69:3X:108:3PE:H372	1.90	1.07
12:1L:519:THR:HG22	69:1L:707:3PE:H232	1.34	1.06
91:4A:609:PGV:H201	66:4L:28:TYR:CD2	1.89	1.06
2:1B:176:TRP:CH2	70:1B:202:PC1:C24	2.39	1.06
47:3P:306:MET:SD	69:3P:514:3PE:H252	1.96	1.06
53:3W:57:LYS:C	53:3W:58:HIS:CD2	2.24	1.06
53:3J:57:LYS:HG3	53:3J:58:HIS:H	1.16	1.06
53:3J:57:LYS:HG2	53:3J:58:HIS:N	1.70	1.06
47:3P:306:MET:HE2	69:3P:514:3PE:H252	1.09	1.06
61:4G:37:LEU:HD22	69:4G:104:3PE:HN2	1.11	1.06
2:1B:177:TYR:HA	70:1B:202:PC1:C26	1.84	1.05
31:1f:28:ARG:NH2	69:1f:103:3PE:C3	2.00	1.05
69:3J:103:3PE:H2C2	69:3J:103:3PE:H2G1	1.31	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3S:201:3PE:H32	69:3S:201:3PE:H232	1.36	1.05
47:3C:305:PRO:O	69:3C:506:3PE:H121	1.56	1.05
69:3P:503:3PE:H241	69:3P:503:3PE:H11	1.24	1.05
24:1Y:87:LEU:CD1	69:1Y:212:3PE:H332	1.87	1.05
39:1n:54:LYS:CD	45:3N:20:ASP:O	1.94	1.05
69:3P:511:3PE:H3A1	69:3P:512:3PE:H392	1.37	1.04
69:1d:206:3PE:H381	69:1f:104:3PE:H2B1	1.26	1.04
31:1f:10:HIS:CE1	69:1f:102:3PE:H232	1.92	1.04
48:3D:232:ARG:HD3	49:3R:237:PRO:HB3	1.37	1.04
51:3G:33:THR:HG22	69:3G:103:3PE:H2	1.39	1.04
91:4A:609:PGV:H201	66:4L:28:TYR:CE2	1.93	1.04
35:1j:38:TRP:CH2	69:1k:101:3PE:C34	2.41	1.03
48:3Q:40:CYS:SG	86:3Q:501:HEC:CBC	2.46	1.03
45:3N:445:ARG:HG2	69:3N:501:3PE:H231	1.34	1.03
48:3Q:37:CYS:SG	86:3Q:501:HEC:CAB	2.47	1.03
75:4B:302:CDL:OA9	63:4I:35:TYR:CE1	2.11	1.03
53:3J:57:LYS:CG	53:3J:58:HIS:N	1.93	1.03
69:1Y:214:3PE:H3H2	75:3P:513:CDL:H142	1.38	1.03
24:1Y:58:TYR:HA	69:1Y:208:3PE:O32	1.57	1.03
24:1Y:108:GLY:HA2	70:1Y:206:PC1:C23	1.89	1.02
47:3C:356:ILE:HG12	69:3C:512:3PE:H2B2	1.38	1.02
47:3P:4:ILE:HD11	69:3P:511:3PE:H112	1.39	1.02
69:3P:508:3PE:H332	75:3P:513:CDL:H131	1.41	1.02
75:3P:513:CDL:H631	75:3T:101:CDL:C34	1.90	1.02
47:3P:249:LEU:HD11	69:3P:520:3PE:H221	1.40	1.02
69:3W:102:3PE:H372	69:3X:101:3PE:H392	1.39	1.02
57:4C:210:ILE:HG23	91:4C:305:PGV:H12	1.41	1.02
12:1L:123:LEU:HD21	75:1L:704:CDL:H351	1.41	1.02
69:1d:206:3PE:H381	69:1f:104:3PE:C2A	1.90	1.02
24:1Y:107:TYR:HD2	69:1Y:213:3PE:O12	1.40	1.02
69:3P:508:3PE:H3I2	75:3P:513:CDL:H441	1.07	1.02
51:3G:44:ARG:NH2	69:3G:105:3PE:C12	2.22	1.01
2:1B:177:TYR:CD1	70:1B:202:PC1:H272	1.94	1.01
12:1L:519:THR:CG2	69:1L:707:3PE:H232	1.90	1.01
46:3B:47:ILE:HD11	46:3B:211:VAL:HG11	1.38	1.01
53:3J:17:ARG:CD	69:3J:103:3PE:C2	2.27	1.01
53:3J:57:LYS:C	53:3J:58:HIS:CG	2.38	1.01
6:1F:362:CYS:SG	71:1F:502:SF4:FE4	1.53	1.01
38:1m:92:PHE:CZ	69:1m:203:3PE:H231	1.94	1.01
10:1J:99:MET:CE	69:1J:203:3PE:H3C1	1.90	1.01
49:3R:172:LYS:HD3	49:3R:214:ILE:HG21	1.39	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:92:PHE:CE1	69:1m:203:3PE:C37	2.44	1.00
46:3B:200:THR:HB	46:3B:227:ARG:HG2	1.43	1.00
69:3P:503:3PE:C1	69:3P:503:3PE:C24	2.20	1.00
69:3P:514:3PE:H121	54:3Y:2:LEU:HD13	1.01	1.00
2:1B:177:TYR:HA	70:1B:202:PC1:H252	1.40	1.00
12:1L:23:ASN:HB3	69:1L:709:3PE:O14	1.62	1.00
47:3C:349:ILE:CD1	69:3C:511:3PE:H222	1.91	1.00
1:1A:23:TRP:NE1	70:1A:202:PC1:O12	1.95	1.00
38:1m:99:PHE:CD2	69:1m:205:3PE:H3G2	1.97	0.99
56:4B:7:LEU:HD12	75:4B:302:CDL:H712	1.00	0.99
13:1M:197:LEU:HB3	82:1Y:203:PGT:H411	1.40	0.99
35:1j:38:TRP:NE1	69:1k:101:3PE:C38	2.26	0.99
53:3J:57:LYS:HG2	53:3J:58:HIS:H	1.23	0.99
69:3J:105:3PE:H2G2	69:3Y:102:3PE:H3B1	1.45	0.99
12:1L:463:PHE:HB2	69:1L:703:3PE:H272	1.43	0.99
12:1L:504:LEU:HD12	69:1L:707:3PE:N	1.76	0.99
69:3P:508:3PE:H3I1	75:3P:513:CDL:H441	1.42	0.99
7:1G:159:CYS:HG	71:1G:802:SF4:FE3	0.72	0.99
54:3X:44:TRP:HZ2	69:3X:108:3PE:H221	1.24	0.98
69:3X:101:3PE:H2B1	69:3X:108:3PE:H2F2	1.43	0.98
40:1o:75:ASN:OD1	69:1o:201:3PE:H252	1.62	0.98
75:3A:501:CDL:H522	69:3A:503:3PE:H272	1.41	0.98
48:3Q:218:LEU:HD21	69:3R:305:3PE:H392	1.45	0.98
31:1f:22:PHE:CD2	69:1f:104:3PE:H372	1.98	0.98
47:3C:349:ILE:HD12	69:3C:511:3PE:H222	1.46	0.98
56:4B:7:LEU:HD12	75:4B:302:CDL:C71	1.93	0.98
69:1Y:214:3PE:H241	69:1Y:214:3PE:H351	1.41	0.98
75:3A:501:CDL:C51	69:3A:503:3PE:H272	1.92	0.98
24:1Y:75:ILE:HG21	69:1Y:214:3PE:H282	1.44	0.98
24:1Y:39:SER:HA	69:1Y:204:3PE:H11	1.45	0.97
51:3G:44:ARG:NH2	69:3G:105:3PE:N	2.11	0.97
12:1L:567:SER:OG	69:1L:705:3PE:C32	2.11	0.97
47:3C:360:LEU:HA	69:3C:512:3PE:H2I2	1.46	0.97
69:3G:108:3PE:H342	69:3G:108:3PE:H251	1.46	0.97
46:3B:201:SER:HB2	46:3B:228:GLY:HA2	1.46	0.97
29:1d:8:ARG:HD3	70:1d:204:PC1:H231	1.00	0.97
69:3P:503:3PE:H12	69:3P:503:3PE:H242	1.44	0.97
69:1N:401:3PE:H292	69:1d:201:3PE:H3A1	1.45	0.97
27:1b:27:LEU:HD11	69:1b:101:3PE:C2F	1.94	0.97
69:1d:201:3PE:C3C	69:1d:201:3PE:C2E	2.43	0.97
9:1I:45:PRO:HD2	26:1a:1:MET:HG3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:77:CYS:HG	71:1I:202:SF4:FE4	0.71	0.96
69:3P:508:3PE:C3I	75:3P:513:CDL:C44	2.43	0.96
55:4A:407:GLN:HE21	91:4A:606:PGV:H062	1.30	0.96
28:1c:34:GLN:HE22	69:1d:203:3PE:H121	1.12	0.96
70:1B:202:PC1:H221	16:1P:275:PHE:CE1	2.01	0.96
69:3P:504:3PE:C2B	69:3P:505:3PE:C38	2.44	0.96
54:3X:44:TRP:CD2	69:3X:108:3PE:H381	2.00	0.96
91:4A:609:PGV:C19	66:4L:28:TYR:CD1	2.48	0.96
12:1L:23:ASN:CB	69:1L:709:3PE:O14	2.13	0.96
69:3R:305:3PE:H3I1	69:3T:103:3PE:H382	1.47	0.96
14:1N:245:MET:HE1	69:1N:401:3PE:H381	1.49	0.95
69:1L:710:3PE:O22	33:1h:26:ARG:NH1	1.98	0.95
24:1Y:5:LEU:HD21	69:1Y:211:3PE:C31	1.95	0.95
24:1Y:76:SER:HA	69:1Y:214:3PE:C22	1.96	0.95
75:1Y:217:CDL:H202	70:3T:102:PC1:H332	1.47	0.95
69:1B:205:3PE:O31	75:1q:202:CDL:C53	2.15	0.95
10:1J:88:THR:OG1	69:1J:201:3PE:H32	1.66	0.95
69:3W:102:3PE:H252	69:3W:102:3PE:H382	1.49	0.95
69:3P:511:3PE:H2E1	69:3P:511:3PE:C2A	1.96	0.95
2:1B:177:TYR:CD1	70:1B:202:PC1:C27	2.49	0.94
2:1B:176:TRP:CZ3	70:1B:202:PC1:C24	2.50	0.94
14:1N:245:MET:CE	69:1N:401:3PE:H381	1.98	0.94
24:1Y:78:GLN:NE2	51:3T:56:TYR:OH	2.00	0.94
29:1d:8:ARG:HD2	70:1d:204:PC1:H252	1.48	0.94
49:3E:164:ASN:HA	49:3E:177:ARG:HB2	1.46	0.94
75:3N:502:CDL:H541	69:3P:511:3PE:H362	1.49	0.94
48:3Q:40:CYS:SG	86:3Q:501:HEC:HBC3	2.06	0.94
91:4A:609:PGV:O04	66:4L:28:TYR:CD1	2.20	0.94
56:4B:7:LEU:CD1	75:4B:302:CDL:C71	2.45	0.94
69:1B:205:3PE:C3	69:1B:205:3PE:H341	1.98	0.94
25:1Z:36:PHE:O	25:1Z:40:ILE:HG12	1.67	0.94
24:1Y:24:SER:HA	69:1Y:208:3PE:H3E2	1.46	0.94
24:1Y:62:SER:OG	69:1Y:208:3PE:C34	2.15	0.94
24:1Y:80:ARG:NH1	69:1Y:212:3PE:O22	2.00	0.94
49:3R:183:GLU:HB3	49:3R:245:ALA:HB2	1.48	0.94
15:1O:188:ASN:HB3	15:1O:191:GLU:HB2	1.49	0.94
29:1d:8:ARG:HG2	70:1d:204:PC1:H242	1.47	0.94
69:3P:514:3PE:C12	54:3Y:2:LEU:HD11	1.88	0.94
10:1J:99:MET:SD	69:1J:203:3PE:H3D2	2.08	0.94
13:1M:54:LEU:HD11	33:1h:96:ILE:HD11	1.50	0.94
35:1j:38:TRP:HE1	69:1k:101:3PE:H382	1.32	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:445:ARG:HG3	75:3N:502:CDL:OB3	1.67	0.94
2:1B:176:TRP:CE3	70:1B:202:PC1:C24	2.50	0.93
5:1E:148:CYS:HG	72:1E:301:FES:FE2	0.73	0.93
53:3J:58:HIS:O	53:3J:60:TYR:N	2.00	0.93
24:1Y:107:TYR:CD2	69:1Y:213:3PE:O12	2.20	0.93
69:3C:513:3PE:H241	69:3C:517:3PE:H351	1.49	0.93
68:4N:40:ASN:OD1	91:4N:101:PGV:O06	1.86	0.93
75:3A:501:CDL:H871	69:3A:503:3PE:H261	1.49	0.93
69:1d:201:3PE:C3C	69:1d:201:3PE:C2F	0.93	0.93
69:1N:401:3PE:H3C2	69:1d:201:3PE:H2C2	1.50	0.93
49:3E:263:TYR:CD1	49:3E:271:VAL:HB	2.04	0.93
49:3R:232:GLY:HA3	49:3R:244:ASP:HA	1.50	0.93
75:3X:103:CDL:H381	69:3X:105:3PE:H3F2	1.49	0.93
70:1H:403:PC1:H252	10:1J:45:LEU:HB3	1.50	0.93
91:4A:608:PGV:H343	75:4B:302:CDL:C87	1.98	0.93
61:4G:37:LEU:HD23	69:4G:104:3PE:H122	1.49	0.93
75:1L:704:CDL:C14	13:1M:361:MET:HE1	1.98	0.93
87:3X:102:PEK:HN2	60:4F:1:ALA:CB	1.82	0.93
69:4G:101:3PE:H321	69:4G:104:3PE:H232	1.51	0.93
75:1g:201:CDL:HA21	33:1h:24:LEU:HD12	1.48	0.93
46:3O:196:GLN:HA	46:3O:227:ARG:HD3	1.50	0.93
69:3P:512:3PE:H292	69:3P:512:3PE:H331	1.51	0.93
69:3W:103:3PE:H351	54:3X:23:MET:HE1	1.51	0.93
24:1Y:80:ARG:HD2	69:1Y:212:3PE:H221	1.50	0.92
75:3A:501:CDL:H473	70:3J:106:PC1:H3G1	1.50	0.92
49:3E:261:PRO:HB2	49:3E:273:VAL:HG11	1.49	0.92
69:1L:709:3PE:H2A1	13:1M:446:LEU:HD11	1.46	0.92
34:1i:83:TYR:CD2	75:1i:201:CDL:H511	2.04	0.92
12:1L:517:SER:HG	69:1L:708:3PE:H11	1.24	0.92
61:4G:37:LEU:CD2	69:4G:104:3PE:HN2	1.50	0.92
7:1G:110:GLN:HG3	7:1G:114:CYS:HA	1.49	0.92
13:1M:105:PHE:HE2	69:1N:401:3PE:H3I1	1.33	0.92
69:1B:205:3PE:H341	69:1B:205:3PE:H31	1.52	0.92
10:1J:99:MET:HE1	69:1J:201:3PE:C3F	1.98	0.92
69:1Y:201:3PE:H261	69:1Y:201:3PE:H3A1	1.49	0.92
38:1m:92:PHE:CE1	69:1m:203:3PE:H271	2.05	0.92
54:3X:44:TRP:CZ2	69:3X:108:3PE:H372	2.04	0.92
69:1m:203:3PE:H251	69:1m:204:3PE:H232	1.50	0.92
1:1A:27:LEU:HG	8:1H:59:GLU:HG3	1.51	0.92
47:3C:352:GLN:HE21	69:3C:511:3PE:H221	1.34	0.91
69:3J:105:3PE:H2E1	69:3Y:102:3PE:H391	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3N:503:3PE:H252	70:3R:303:PC1:H222	1.50	0.91
13:1M:33:LEU:HB3	69:1f:103:3PE:H3F1	1.51	0.91
35:1j:38:TRP:CH2	69:1k:101:3PE:H371	2.05	0.91
51:3G:44:ARG:NH2	69:3G:105:3PE:H121	1.86	0.91
69:3Y:105:3PE:H2F2	69:3Y:105:3PE:H3F2	1.53	0.91
2:1B:176:TRP:CE2	70:1B:202:PC1:H242	2.05	0.91
16:1P:275:PHE:O	16:1P:276:GLU:O	1.89	0.91
34:1i:83:TYR:CE2	75:1i:201:CDL:H511	2.05	0.91
35:1j:38:TRP:CE2	69:1k:101:3PE:C38	2.52	0.91
53:3J:17:ARG:HD3	69:3J:103:3PE:O21	1.71	0.91
12:1L:504:LEU:HD12	69:1L:707:3PE:HN3	1.27	0.91
69:1d:206:3PE:C38	69:1f:104:3PE:C2A	2.48	0.91
46:3B:124:LEU:HD12	46:3B:223:PHE:HB2	1.53	0.91
53:3J:54:LYS:HA	53:3J:57:LYS:HE2	1.53	0.91
47:3P:306:MET:HE1	69:3P:514:3PE:H272	1.53	0.91
2:1B:176:TRP:C	70:1B:202:PC1:H252	1.95	0.90
69:1L:709:3PE:H371	75:1i:201:CDL:H781	1.53	0.90
31:1f:14:ILE:CD1	69:1f:101:3PE:H2B2	2.00	0.90
47:3P:249:LEU:HD12	69:3P:520:3PE:H2	1.50	0.90
38:1m:87:LEU:CD1	69:1m:202:3PE:H251	2.01	0.90
12:1L:66:TRP:CD1	69:1L:702:3PE:H321	2.06	0.90
49:3E:273:VAL:HG23	49:3E:274:GLY:H	1.33	0.90
69:3G:104:3PE:H271	69:3G:104:3PE:H372	1.52	0.90
7:1G:55:CYS:HG	72:1G:803:FES:FE2	0.74	0.90
47:3C:296:ALA:HB1	69:3C:511:3PE:H3G2	1.52	0.90
49:3E:217:CYS:HB3	49:3E:221:GLY:HA2	1.53	0.90
51:3G:44:ARG:HH22	69:3G:105:3PE:H121	1.36	0.90
8:1H:173:TRP:HE1	70:1H:404:PC1:C11	1.84	0.90
24:1Y:38:TYR:CE2	69:1Y:204:3PE:H372	2.06	0.90
48:3Q:144:ARG:HG2	48:3Q:147:LEU:HD22	1.54	0.90
69:3N:501:3PE:H2C1	75:3N:502:CDL:H581	1.52	0.90
55:4A:92:MET:HE3	55:4A:163:ASN:HD22	1.36	0.90
69:1B:205:3PE:O31	75:1q:202:CDL:H532	1.71	0.90
69:1d:206:3PE:C38	69:1f:104:3PE:C2B	2.40	0.90
38:1m:87:LEU:HD12	69:1m:202:3PE:C25	2.02	0.90
11:1K:15:ALA:CB	11:1K:36:MET:HG3	2.02	0.89
11:1K:15:ALA:HB3	11:1K:36:MET:HG3	1.54	0.89
29:1d:34:MET:HE2	29:1d:34:MET:HA	1.52	0.89
55:4A:22:PHE:HD1	91:4A:609:PGV:H12	1.37	0.89
69:1B:205:3PE:C34	69:1B:205:3PE:H31	2.01	0.89
69:1L:709:3PE:C2E	75:1i:201:CDL:H152	2.03	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3C:507:3PE:H282	69:3C:508:3PE:H261	1.52	0.89
53:3J:58:HIS:C	53:3J:60:TYR:N	2.29	0.89
48:3D:232:ARG:HH11	49:3R:237:PRO:HB2	1.38	0.89
24:1Y:75:ILE:CG2	69:1Y:214:3PE:H261	2.02	0.89
75:3N:502:CDL:H122	75:3N:502:CDL:HB32	1.54	0.89
2:1B:176:TRP:CZ3	70:1B:202:PC1:H262	2.08	0.89
38:1m:92:PHE:CD1	69:1m:203:3PE:H371	2.07	0.89
2:1B:177:TYR:CA	70:1B:202:PC1:H252	2.02	0.89
24:1Y:87:LEU:HD22	69:1Y:212:3PE:O32	1.73	0.89
12:1L:570:GLN:HB2	69:1L:705:3PE:H241	1.55	0.89
14:1N:325:LEU:N	75:1d:205:CDL:OA4	2.05	0.89
38:1m:24:ILE:O	45:3N:227:ALA:HB1	1.71	0.89
13:1M:10:MET:HE2	69:1f:104:3PE:H382	1.52	0.89
24:1Y:27:ILE:CB	69:1Y:208:3PE:H3D2	2.03	0.89
24:1Y:105:ARG:NH1	70:1Y:207:PC1:P	2.46	0.89
69:1f:102:3PE:H272	69:1g:202:3PE:H392	1.52	0.89
75:1g:201:CDL:H231	69:1g:202:3PE:H3E1	1.53	0.89
39:1n:54:LYS:HD3	45:3N:20:ASP:O	1.71	0.89
69:3N:501:3PE:H2F2	69:3N:503:3PE:H2G2	1.52	0.89
54:3X:47:TYR:HA	69:3X:101:3PE:H31	1.55	0.89
1:1A:27:LEU:HD11	8:1H:60:PRO:HD2	1.53	0.88
69:1L:703:3PE:H2	40:1o:77:LEU:HD11	0.93	0.88
91:4A:609:PGV:O03	66:4L:28:TYR:CZ	2.24	0.88
69:3E:302:3PE:H332	69:3E:302:3PE:H11	1.54	0.88
24:1Y:95:ALA:HB2	70:1Y:207:PC1:H3C1	1.53	0.88
27:1b:26:GLY:HA3	69:1b:101:3PE:H2C2	1.56	0.88
69:1d:201:3PE:C3F	69:1d:201:3PE:C2F	2.51	0.88
49:3R:235:TYR:HA	49:3R:242:HIS:CA	2.03	0.88
54:3Y:41:ILE:CD1	69:3Y:105:3PE:H371	2.03	0.88
8:1H:244:GLY:O	70:1H:404:PC1:H111	1.72	0.88
12:1L:279:CYS:SG	69:1L:712:3PE:H2H2	2.14	0.88
75:3A:501:CDL:H522	69:3A:503:3PE:C27	2.03	0.88
24:1Y:5:LEU:CD2	69:1Y:211:3PE:H321	2.04	0.88
48:3Q:118:ARG:HG3	48:3Q:194:SER:HB3	1.54	0.88
2:1B:176:TRP:CE3	70:1B:202:PC1:H231	2.08	0.88
69:3Y:101:3PE:H241	69:3Y:101:3PE:H321	1.56	0.88
54:3Y:33:VAL:HG21	69:3Y:105:3PE:H2G1	1.55	0.88
91:4A:609:PGV:H32	91:4A:609:PGV:H212	1.54	0.88
57:4C:62:ILE:HG13	91:4C:305:PGV:H21	1.55	0.88
24:1Y:124:VAL:HG22	69:1Y:211:3PE:H282	1.55	0.88
45:3N:141:ASN:HA	49:3V:47:ARG:HH21	1.39	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1M:501:PC1:H111	75:1i:201:CDL:H112	1.55	0.87
47:3C:284:ILE:HD12	69:3C:512:3PE:H352	0.88	0.87
51:3G:44:ARG:HH21	69:3G:105:3PE:HN1	1.22	0.87
75:1L:704:CDL:H512	75:1L:704:CDL:H711	1.56	0.87
14:1N:257:LEU:HD21	69:1N:401:3PE:H2D1	1.55	0.87
12:1L:485:TYR:HB3	91:4J:101:PGV:H201	1.55	0.87
12:1L:567:SER:HG	69:1L:705:3PE:H322	1.05	0.87
38:1m:24:ILE:O	45:3N:227:ALA:HB2	1.72	0.87
54:3X:44:TRP:CE3	69:3X:108:3PE:H381	2.09	0.87
1:1A:108:GLN:NE2	69:1A:203:3PE:H251	1.90	0.87
12:1L:24:SER:HA	69:1L:710:3PE:P	2.14	0.87
29:1d:8:ARG:CD	70:1d:204:PC1:H231	1.97	0.87
31:1f:10:HIS:CE1	69:1f:102:3PE:O22	2.28	0.87
69:3C:507:3PE:H241	69:3C:508:3PE:H242	1.54	0.87
8:1H:99:ASN:CG	70:1H:403:PC1:C15	2.48	0.87
91:4A:609:PGV:H261	66:4L:28:TYR:HB3	1.56	0.87
69:3G:103:3PE:H251	69:3G:108:3PE:H241	1.55	0.87
69:3Y:105:3PE:H2C1	69:3Y:105:3PE:H3H1	1.56	0.87
12:1L:566:THR:HG21	69:1L:705:3PE:H381	1.55	0.86
75:1L:704:CDL:H622	13:1M:448:THR:HG21	1.57	0.86
75:1g:201:CDL:H651	75:1g:201:CDL:H392	1.57	0.86
69:3P:508:3PE:H3I2	75:3P:513:CDL:C44	2.00	0.86
70:1B:202:PC1:C2A	70:1B:202:PC1:C24	2.52	0.86
12:1L:524:ASN:HD21	39:1n:77:GLN:HG2	1.39	0.86
1:1A:5:LEU:HD11	8:1H:3:MET:HE1	1.54	0.86
69:3C:516:3PE:H221	69:3Y:107:3PE:H322	1.56	0.86
49:3E:241:SER:CA	49:3E:252:GLY:HA3	2.03	0.86
47:3P:306:MET:HE1	69:3P:514:3PE:H261	1.07	0.86
1:1A:44:MET:HE3	1:1A:46:SER:H	1.40	0.86
69:1A:201:3PE:H2D1	8:1H:302:MET:HE1	1.57	0.86
8:1H:173:TRP:HE1	70:1H:404:PC1:H111	1.40	0.86
14:1N:257:LEU:CD2	69:1N:401:3PE:H2D1	2.06	0.86
16:1P:99:TRP:CZ2	16:1P:276:GLU:HG3	2.11	0.86
2:1B:176:TRP:CE2	70:1B:202:PC1:C22	2.58	0.86
2:1B:177:TYR:HD1	70:1B:202:PC1:H282	1.39	0.86
69:1d:201:3PE:H2H1	69:1d:201:3PE:C3E	2.04	0.86
69:3C:503:3PE:H2B2	69:3C:503:3PE:H361	1.55	0.86
51:3G:63:TRP:CE2	69:3G:110:3PE:H2	2.11	0.86
69:3P:503:3PE:H3D2	69:3P:503:3PE:H2F2	1.55	0.86
45:3A:250:LEU:HD12	49:3I:44:ASP:HB2	1.56	0.86
47:3C:287:LYS:HB2	69:3C:513:3PE:C12	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:467:ILE:HD11	69:1L:703:3PE:H221	1.57	0.86
12:1L:534:HIS:HB3	69:1L:701:3PE:H31	1.58	0.86
69:3P:512:3PE:H391	69:3P:512:3PE:H3D1	1.56	0.86
70:1B:202:PC1:H241	70:1B:202:PC1:H2A1	1.56	0.85
24:1Y:27:ILE:HG22	69:1Y:208:3PE:H2F1	1.58	0.85
24:1Y:105:ARG:NH1	70:1Y:207:PC1:O13	2.09	0.85
29:1d:8:ARG:CD	70:1d:204:PC1:H252	2.06	0.85
31:1f:21:VAL:HG21	69:1f:104:3PE:H3G2	1.58	0.85
69:3N:501:3PE:H3B1	47:3P:14:ILE:CD1	2.06	0.85
69:3P:503:3PE:H241	69:3P:503:3PE:H12	0.99	0.85
69:3P:520:3PE:H3G1	69:3Q:504:3PE:H3E1	1.56	0.85
54:3Y:5:PHE:HZ	69:3Y:107:3PE:H2	1.40	0.85
75:4C:306:CDL:H141	75:4C:306:CDL:H561	1.56	0.85
49:3R:235:TYR:CA	49:3R:242:HIS:HA	2.06	0.85
28:1c:30:TYR:HE2	69:1d:203:3PE:H341	0.86	0.85
47:3C:286:ASN:HD21	69:3C:513:3PE:H12	1.38	0.85
75:1N:402:CDL:HB62	69:1e:201:3PE:H12	1.57	0.85
15:1O:133:VAL:HG22	15:1O:202:ILE:HG23	1.55	0.85
53:3J:17:ARG:CD	69:3J:103:3PE:O11	2.24	0.85
54:3Y:6:LEU:CD2	69:3Y:107:3PE:H2D1	2.06	0.85
28:1c:30:TYR:CD2	69:1d:203:3PE:H341	2.11	0.85
69:3P:508:3PE:H3I1	75:3P:513:CDL:C44	2.06	0.85
69:3X:108:3PE:H332	69:4G:104:3PE:H352	1.58	0.85
13:1M:10:MET:CE	69:1f:104:3PE:H382	2.07	0.85
24:1Y:107:TYR:HD2	69:1Y:213:3PE:P	1.99	0.85
28:1c:30:TYR:CE2	69:1d:203:3PE:C34	2.47	0.85
69:3C:508:3PE:H3F2	75:3F:201:CDL:H261	1.59	0.85
75:3Y:106:CDL:H112	75:3Y:106:CDL:H522	1.58	0.85
93:4B:303:PSC:H202	63:4I:18:ARG:HG3	1.58	0.85
69:1J:201:3PE:H2G2	69:1J:201:3PE:H3B1	1.57	0.85
75:1L:704:CDL:H142	13:1M:361:MET:CE	2.02	0.85
51:3G:44:ARG:NH1	69:3G:107:3PE:H112	1.90	0.85
29:1d:60:ARG:NH1	75:1d:205:CDL:OB3	2.10	0.85
13:1M:105:PHE:CE2	69:1N:401:3PE:H3I1	2.12	0.85
49:3E:155:LYS:HG3	49:3E:274:GLY:OXT	1.76	0.85
48:3Q:218:LEU:HD23	69:3R:305:3PE:H372	1.59	0.85
2:1B:44:SER:HB2	8:1H:54:LYS:HD3	1.56	0.84
49:3R:214:ILE:HG12	49:3R:261:PRO:HG3	1.57	0.84
69:1B:205:3PE:O31	75:1q:202:CDL:C52	2.05	0.84
69:3N:503:3PE:H2D1	69:3R:304:3PE:H2G1	1.59	0.84
55:4A:109:PHE:HB3	91:4A:609:PGV:C17	2.02	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3C:517:3PE:H321	69:4G:101:3PE:H251	1.59	0.84
75:3N:502:CDL:H762	69:3N:503:3PE:H2B1	1.57	0.84
69:3Y:103:3PE:H282	69:3Y:103:3PE:H362	1.56	0.84
75:1H:401:CDL:HB61	75:1H:401:CDL:C32	2.07	0.84
70:1H:402:PC1:H3F1	27:1b:24:ILE:CD1	2.08	0.84
31:1f:10:HIS:ND1	69:1f:102:3PE:C23	2.39	0.84
56:4B:61:VAL:HG11	93:4B:303:PSC:H52	1.57	0.84
47:3C:296:ALA:HB1	69:3C:511:3PE:C3G	2.07	0.84
47:3C:356:ILE:HG12	69:3C:512:3PE:C2B	2.08	0.84
45:3N:14:THR:HG21	45:3N:389:ARG:HB3	1.60	0.84
51:3T:30:PHE:H	69:3T:103:3PE:H2G2	1.41	0.84
69:3Y:107:3PE:H32	69:3Y:107:3PE:H242	1.58	0.84
55:4A:25:TRP:HB2	91:4A:609:PGV:H291	1.59	0.84
69:1m:202:3PE:H351	51:3T:34:ILE:HD12	1.59	0.84
49:3R:128:ALA:HB1	69:3R:302:3PE:H361	1.58	0.84
93:4B:303:PSC:C07	63:4I:14:ALA:HB2	2.06	0.84
35:1j:38:TRP:HH2	69:1k:101:3PE:H341	1.05	0.84
75:4B:302:CDL:OA9	63:4I:35:TYR:HD1	1.57	0.84
1:1A:108:GLN:HE22	69:1A:203:3PE:C25	1.91	0.84
75:1H:401:CDL:HB61	75:1H:401:CDL:H322	1.60	0.84
12:1L:463:PHE:CB	69:1L:703:3PE:H272	2.07	0.84
24:1Y:62:SER:OG	69:1Y:208:3PE:H322	1.78	0.84
38:1m:92:PHE:HE1	69:1m:203:3PE:C36	1.91	0.84
69:3N:503:3PE:H3H2	69:3R:304:3PE:H2E1	1.59	0.84
54:3Y:23:MET:HE2	69:3Y:101:3PE:H342	1.60	0.84
24:1Y:75:ILE:CG2	69:1Y:214:3PE:H282	2.06	0.83
49:3E:242:HIS:HB2	49:3E:251:LYS:HB3	1.58	0.83
53:3J:46:HIS:CD2	69:3J:101:3PE:H322	2.13	0.83
45:3N:436:ARG:HD3	47:3P:222:PRO:HD3	1.58	0.83
46:3O:303:VAL:HG21	46:3O:336:VAL:HG22	1.60	0.83
55:4A:1:FME:CN	91:4A:609:PGV:H1	1.76	0.83
29:1d:8:ARG:CG	70:1d:204:PC1:H242	2.08	0.83
69:3J:104:3PE:H2G1	69:3J:105:3PE:H351	1.58	0.83
24:1Y:122:ALA:CB	70:1Y:202:PC1:H351	2.08	0.83
11:1K:26:LEU:HB3	11:1K:78:LEU:HD12	1.58	0.83
24:1Y:5:LEU:HD21	69:1Y:211:3PE:O32	1.77	0.83
69:3A:503:3PE:H2E2	69:3Y:107:3PE:H3F2	1.59	0.83
54:3X:22:SER:OG	69:3X:106:3PE:H352	1.77	0.83
69:1d:206:3PE:H381	69:1f:104:3PE:H2A2	1.61	0.83
69:3G:101:3PE:H3D1	69:3G:101:3PE:H382	1.59	0.83
69:3W:103:3PE:H121	69:3W:103:3PE:H2	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
68:4N:40:ASN:HB3	68:4N:43:VAL:HG22	1.59	0.83
69:1B:205:3PE:H342	69:1B:205:3PE:H32	0.84	0.83
24:1Y:75:ILE:CG2	69:1Y:201:3PE:C27	2.57	0.83
69:3A:503:3PE:H111	75:3Y:106:CDL:H511	1.59	0.83
53:3W:57:LYS:C	53:3W:58:HIS:HD2	1.83	0.83
10:1J:99:MET:CE	69:1J:201:3PE:C3F	2.54	0.83
33:1h:73:ARG:NE	70:1h:202:PC1:O14	2.10	0.83
38:1m:92:PHE:CD1	69:1m:203:3PE:C27	2.61	0.83
24:1Y:62:SER:HB3	69:1Y:208:3PE:H371	0.84	0.83
47:3C:352:GLN:NE2	69:3C:511:3PE:C22	2.40	0.83
69:3G:105:3PE:H122	69:3G:107:3PE:N	1.94	0.83
54:3X:15:ARG:NH1	87:3X:102:PEK:O13	2.11	0.83
61:4G:37:LEU:HD21	69:4G:104:3PE:N	1.74	0.83
1:1A:108:GLN:HE22	69:1A:203:3PE:H251	1.44	0.83
14:1N:7:THR:HG21	75:1N:402:CDL:H341	1.59	0.83
91:4A:609:PGV:O04	66:4L:28:TYR:HE1	1.62	0.83
28:1c:22:GLY:HA3	75:1d:205:CDL:H872	1.61	0.82
40:1o:77:LEU:CB	69:1o:201:3PE:H261	2.09	0.82
45:3A:121:SER:HB3	45:3A:123:GLU:HG3	1.62	0.82
53:3J:17:ARG:NE	69:3J:103:3PE:H2	1.72	0.82
2:1B:177:TYR:CA	70:1B:202:PC1:C25	2.55	0.82
13:1M:40:SER:HB3	70:1h:203:PC1:H332	1.61	0.82
69:3R:304:3PE:H392	70:3X:104:PC1:H2D2	1.59	0.82
75:3T:101:CDL:H531	75:3T:101:CDL:H711	1.59	0.82
69:1L:710:3PE:H221	33:1h:26:ARG:HH11	0.67	0.82
33:1h:78:THR:O	70:1h:203:PC1:H153	1.78	0.82
69:3T:103:3PE:H2	69:3T:103:3PE:H2E1	1.60	0.82
13:1M:92:LYS:O	13:1M:96:ILE:HG12	1.80	0.82
27:1b:23:ALA:HB1	69:1b:101:3PE:C2G	2.09	0.82
69:3N:503:3PE:H272	70:3R:303:PC1:H241	1.61	0.82
24:1Y:62:SER:CB	69:1Y:208:3PE:H341	2.10	0.82
75:3F:201:CDL:H221	69:3G:109:3PE:H352	1.62	0.82
51:3G:56:VAL:CG2	69:3G:109:3PE:H2A2	2.07	0.82
69:3Y:101:3PE:H2H2	69:3Y:104:3PE:H3B2	1.61	0.82
24:1Y:117:MET:HG2	70:1Y:206:PC1:H3C2	1.62	0.82
36:1k:34:LYS:NZ	64:4J:17:ASP:OD2	2.11	0.82
49:3E:129:ALA:HA	69:3E:303:3PE:H3C2	1.61	0.82
70:1H:404:PC1:H3I1	69:1Z:201:3PE:H272	1.62	0.82
69:3C:515:3PE:H232	69:3P:514:3PE:H341	1.61	0.82
69:3C:512:3PE:H3A2	69:3C:513:3PE:H2C1	1.62	0.82
69:3T:103:3PE:N	69:3T:103:3PE:H11	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:118:GLN:HE22	45:3A:216:PHE:HA	1.45	0.81
45:3N:356:ARG:O	45:3N:360:ILE:HG13	1.79	0.81
69:1A:201:3PE:H3A1	69:1b:101:3PE:H2A2	1.62	0.81
75:1g:201:CDL:H791	33:1h:35:PRO:HG3	1.60	0.81
69:3C:511:3PE:H392	69:3C:512:3PE:H2B1	1.62	0.81
2:1B:176:TRP:CE2	70:1B:202:PC1:H222	2.15	0.81
70:1H:402:PC1:H2B1	9:1I:34:LEU:HD21	1.62	0.81
69:1d:206:3PE:H372	69:1f:104:3PE:H292	1.62	0.81
40:1o:77:LEU:HD12	69:1o:201:3PE:C26	2.11	0.81
47:3C:287:LYS:HB2	69:3C:513:3PE:H122	1.61	0.81
49:3E:179:ARG:HD3	49:3E:211:VAL:HB	1.60	0.81
49:3E:235:TYR:HA	49:3E:243:TYR:H	1.45	0.81
49:3E:239:HIS:O	72:3E:301:FES:FE2	1.31	0.81
54:3X:44:TRP:CZ3	69:3X:108:3PE:C37	2.64	0.81
91:4C:303:PGV:H302	91:4C:303:PGV:H162	1.62	0.81
2:1B:177:TYR:CD1	70:1B:202:PC1:C28	2.63	0.81
8:1H:77:LEU:CD1	70:1H:403:PC1:C3C	2.59	0.81
14:1N:246:VAL:HG11	69:1N:401:3PE:H2C2	1.63	0.81
24:1Y:27:ILE:CG2	69:1Y:208:3PE:H2F1	2.11	0.81
45:3A:204:GLU:HG2	45:3A:207:GLN:H	1.45	0.81
47:3C:215:MET:HG2	50:3F:71:VAL:HG13	1.60	0.81
53:3J:47:ILE:HD11	69:3J:101:3PE:H271	1.63	0.81
75:3N:502:CDL:H861	75:3X:103:CDL:H811	1.63	0.81
91:4C:302:PGV:H291	75:4C:307:CDL:H402	1.60	0.81
91:4G:102:PGV:H251	91:4G:102:PGV:H132	1.63	0.81
51:3G:63:TRP:NE1	69:3G:110:3PE:H2	1.96	0.81
55:4A:419:VAL:HG22	91:4A:608:PGV:H131	1.61	0.81
24:1Y:76:SER:HA	69:1Y:214:3PE:H222	1.62	0.81
47:3C:355:SER:HB2	69:3C:511:3PE:H372	1.63	0.81
69:3D:503:3PE:H222	69:3G:101:3PE:H222	1.61	0.81
56:4B:59:GLN:HE22	68:4N:12:HIS:HA	1.45	0.81
8:1H:96:ILE:HG23	25:1Z:144:THR:HB	1.61	0.81
10:1J:87:LYS:O	69:1J:201:3PE:H322	1.81	0.81
49:3E:266:THR:HB	49:3E:270:LEU:HG	1.63	0.80
54:3X:44:TRP:CD2	69:3X:108:3PE:C38	2.63	0.80
31:1f:21:VAL:HG21	69:1f:104:3PE:C3G	2.10	0.80
75:3A:501:CDL:C1	69:3A:503:3PE:H12	2.11	0.80
46:3B:299:VAL:HG21	46:3B:309:VAL:HG11	1.64	0.80
69:3P:520:3PE:H361	69:3P:520:3PE:H2A2	1.63	0.80
1:1A:27:LEU:HD22	70:1A:202:PC1:H152	1.62	0.80
24:1Y:32:GLY:HA2	24:1Y:35:VAL:CG1	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:444:LEU:CD2	69:3N:503:3PE:H112	2.11	0.80
55:4A:21:LEU:CD1	91:4A:609:PGV:H62	2.11	0.80
31:1f:21:VAL:HG12	69:1f:103:3PE:H331	1.63	0.80
75:3N:502:CDL:H511	69:3P:511:3PE:O32	1.80	0.80
91:4A:609:PGV:C20	66:4L:28:TYR:CD1	2.64	0.80
32:1g:56:TRP:HB3	69:1g:202:3PE:H241	1.62	0.80
49:3E:174:LEU:HD13	49:3E:214:ILE:HD13	1.62	0.80
47:3P:29:SER:OG	75:3P:513:CDL:OA9	2.00	0.80
49:3R:162:GLY:H	49:3R:178:HIS:HB3	1.47	0.80
2:1B:177:TYR:HD1	70:1B:202:PC1:C28	1.95	0.80
69:1f:104:3PE:H242	69:1f:104:3PE:H332	1.64	0.80
48:3Q:218:LEU:CD2	69:3R:305:3PE:H392	2.11	0.80
54:3X:44:TRP:HZ2	69:3X:108:3PE:C22	1.94	0.80
10:1J:91:GLY:HA3	69:1J:201:3PE:H362	1.64	0.80
12:1L:541:ASN:OD1	69:1L:701:3PE:H291	1.81	0.80
47:3P:10:LEU:HD23	69:3P:512:3PE:H382	1.64	0.80
54:3Y:6:LEU:HD23	69:3Y:107:3PE:H2D1	1.63	0.80
47:3P:92:ILE:CD1	69:3P:519:3PE:H291	2.09	0.80
47:3C:286:ASN:ND2	69:3C:512:3PE:O12	2.15	0.80
58:4D:126:MET:HG3	63:4I:68:ILE:HD13	1.62	0.80
8:1H:204:GLU:HG2	8:1H:279:ARG:HH22	1.46	0.79
37:1l:111:PHE:CG	69:1l:203:3PE:H281	2.14	0.79
53:3J:17:ARG:HD2	69:3J:103:3PE:P	2.22	0.79
69:3J:105:3PE:C2G	69:3Y:102:3PE:H391	2.12	0.79
75:4C:306:CDL:H581	75:4C:306:CDL:H761	1.62	0.79
54:3X:14:ALA:O	54:3X:18:ILE:HG13	1.82	0.79
91:4A:609:PGV:C20	66:4L:28:TYR:CG	2.65	0.79
1:1A:49:LEU:HD12	8:1H:126:LYS:HG3	1.62	0.79
1:1A:23:TRP:CD2	70:1A:202:PC1:O12	2.35	0.79
24:1Y:80:ARG:HH11	69:1Y:212:3PE:C21	1.96	0.79
24:1Y:120:THR:HG21	70:1Y:206:PC1:C3F	2.12	0.79
12:1L:123:LEU:CD2	75:1L:704:CDL:H351	2.13	0.79
69:3C:510:3PE:H12	69:3C:510:3PE:H122	0.83	0.79
45:3N:18:GLN:HG3	45:3N:24:ARG:HG3	1.64	0.79
70:1B:202:PC1:C22	16:1P:275:PHE:HE1	1.94	0.79
69:1d:201:3PE:C3D	69:1d:201:3PE:C2H	2.61	0.79
69:1h:204:3PE:H262	69:1h:204:3PE:H221	1.65	0.79
69:3G:106:3PE:H351	69:3G:107:3PE:H321	1.63	0.79
53:3J:24:THR:HG23	69:3J:103:3PE:H3D2	1.65	0.79
13:1M:216:LEU:HD23	13:1M:291:VAL:HG22	1.63	0.79
24:1Y:76:SER:HA	69:1Y:214:3PE:H221	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:79:VAL:HG11	69:1Y:214:3PE:O31	1.82	0.79
69:1d:206:3PE:C37	69:1f:104:3PE:C2B	2.57	0.79
75:1g:201:CDL:H391	33:1h:32:THR:CG2	2.11	0.79
75:1g:201:CDL:H711	33:1h:27:PHE:CD1	2.17	0.79
45:3A:79:VAL:HA	45:3A:82:MET:HE2	1.65	0.79
12:1L:504:LEU:HD21	64:4J:30:ILE:HD11	1.65	0.79
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.65	0.79
69:1m:201:3PE:H12	69:1m:201:3PE:H121	1.64	0.79
4:1D:346:ILE:HG23	7:1G:117:GLN:HG2	1.65	0.79
69:1L:707:3PE:H12	69:1L:707:3PE:H122	1.62	0.79
24:1Y:24:SER:CA	69:1Y:208:3PE:H3E2	2.12	0.79
69:3A:502:3PE:H391	69:3A:502:3PE:H3D2	1.65	0.79
87:3X:102:PEK:HN2	60:4F:1:ALA:HB2	1.47	0.79
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.18	0.78
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.65	0.78
69:3X:101:3PE:H2C1	69:3X:106:3PE:H3I2	1.65	0.78
91:4C:302:PGV:H292	75:4C:307:CDL:C40	2.11	0.78
61:4G:69:LEU:HD12	87:4G:103:PEK:H231	1.64	0.78
13:1M:29:VAL:CG1	69:1g:202:3PE:H2D2	2.13	0.78
69:3A:503:3PE:H122	69:3C:516:3PE:N	1.99	0.78
47:3P:4:ILE:CD1	69:3P:511:3PE:H112	2.13	0.78
75:3A:501:CDL:H752	69:3A:502:3PE:H2D2	1.65	0.78
69:3C:512:3PE:H32	69:3C:513:3PE:H222	1.66	0.78
69:3N:501:3PE:H112	69:3P:511:3PE:H122	1.64	0.78
47:3P:300:ILE:HA	47:3P:303:LEU:HD23	1.64	0.78
69:3P:505:3PE:H221	69:3P:518:3PE:H31	1.64	0.78
69:1N:401:3PE:H2E2	69:1N:401:3PE:H3G2	1.65	0.78
49:3R:200:HIS:HB3	49:3R:203:GLU:HB3	1.63	0.78
56:4B:35:SER:CB	75:4B:302:CDL:H402	2.12	0.78
7:1G:114:CYS:O	7:1G:115:ASP:HB2	1.83	0.78
12:1L:55:MET:HE1	69:1o:201:3PE:H2I3	1.65	0.78
12:1L:471:ASN:OD1	69:1o:201:3PE:H2F2	1.83	0.78
69:1f:102:3PE:H281	69:1g:202:3PE:H3D2	1.65	0.78
69:3C:506:3PE:H3D2	69:3C:512:3PE:H2H1	1.64	0.78
69:3G:105:3PE:H122	69:3G:107:3PE:HN1	1.46	0.78
47:3P:249:LEU:HD11	69:3P:520:3PE:H2	1.64	0.78
69:1d:206:3PE:C37	69:1f:104:3PE:H292	2.14	0.78
69:3X:107:3PE:H232	69:4G:101:3PE:H122	1.65	0.78
15:1O:77:CYS:SG	15:1O:96:LEU:HA	2.24	0.78
75:4C:307:CDL:CA7	64:4J:1:LEU:HD23	2.13	0.78
70:1M:501:PC1:H321	75:1i:201:CDL:H111	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1d:201:3PE:H3D1	69:1d:201:3PE:C2H	2.13	0.78
69:1m:203:3PE:H381	69:1m:203:3PE:H2C1	1.65	0.78
69:3J:103:3PE:H2C2	69:3J:103:3PE:C2G	2.12	0.78
8:1H:81:LEU:HA	8:1H:84:THR:HG22	1.65	0.78
69:3C:510:3PE:H12	69:3C:510:3PE:C11	2.11	0.78
48:3D:121:TYR:HA	48:3D:125:CYS:SG	2.24	0.78
69:3J:105:3PE:C2E	69:3Y:102:3PE:H391	2.14	0.78
13:1M:195:MET:HG3	82:1Y:203:PGT:O31	1.84	0.77
69:1Y:201:3PE:C33	51:3T:56:TYR:HD1	1.96	0.77
75:3A:501:CDL:H512	69:3A:503:3PE:H272	1.66	0.77
49:3R:160:PRO:HD2	49:3R:163:LYS:HB3	1.65	0.77
69:3R:305:3PE:H3G2	69:3T:103:3PE:H3I3	1.66	0.77
69:3C:516:3PE:H2A2	69:3Y:107:3PE:H3D1	1.66	0.77
2:1B:177:TYR:CD1	70:1B:202:PC1:H282	2.19	0.77
69:1B:204:3PE:H2H1	69:1B:204:3PE:H2D2	1.66	0.77
38:1m:92:PHE:CE2	69:1m:203:3PE:C23	2.67	0.77
75:3A:501:CDL:H851	69:3A:503:3PE:H282	1.66	0.77
69:3G:110:3PE:H242	69:3G:110:3PE:H282	1.66	0.77
69:3Q:504:3PE:H3I1	69:3T:103:3PE:H3G2	1.67	0.77
87:4G:103:PEK:H41	87:4G:103:PEK:H101	1.66	0.77
2:1B:176:TRP:CZ2	70:1B:202:PC1:C22	2.67	0.77
24:1Y:39:SER:HA	69:1Y:204:3PE:C1	2.14	0.77
69:1o:201:3PE:H232	69:1o:201:3PE:H322	1.65	0.77
75:1q:202:CDL:H792	75:1q:202:CDL:H322	1.66	0.77
47:3C:103:TYR:O	47:3C:315:MET:HG3	1.83	0.77
49:3E:128:ALA:HB1	69:3E:303:3PE:H361	1.65	0.77
49:3E:241:SER:HA	49:3E:252:GLY:CA	2.06	0.77
46:3O:56:ARG:HD2	46:3O:103:GLU:HG2	1.66	0.77
55:4A:102:PHE:HZ	91:4A:609:PGV:H91	1.49	0.77
55:4A:208:MET:HE3	57:4C:100:ALA:HB2	1.65	0.77
2:1B:177:TYR:CB	70:1B:202:PC1:H261	2.15	0.77
69:1L:702:3PE:H291	34:1i:80:ILE:HG23	1.65	0.77
75:1N:402:CDL:H771	69:1e:201:3PE:H2G1	1.66	0.77
24:1Y:27:ILE:CG2	69:1Y:208:3PE:C2F	2.62	0.77
28:1c:26:PHE:CE2	75:1d:205:CDL:H802	2.20	0.77
31:1f:21:VAL:HG23	69:1f:104:3PE:H3E2	1.64	0.77
51:3G:47:ILE:HG23	51:3G:48:LEU:HD13	1.67	0.77
49:3R:178:HIS:CE1	49:3R:209:GLU:HB3	2.19	0.77
31:1f:21:VAL:CG2	69:1f:104:3PE:C3E	2.62	0.77
31:1f:25:TYR:OH	69:1f:104:3PE:O21	2.02	0.77
49:3E:213:LEU:HA	49:3E:261:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:227:ASN:H	49:3R:234:TYR:HD1	1.32	0.77
91:4A:609:PGV:C20	66:4L:28:TYR:CD2	2.67	0.77
1:1A:103:ALA:CB	69:1b:101:3PE:H351	2.15	0.77
2:1B:34:ASP:HB3	2:1B:174:ARG:HH21	1.50	0.77
69:1Y:214:3PE:H3H2	75:3P:513:CDL:H171	1.67	0.77
54:3Y:5:PHE:CZ	69:3Y:107:3PE:H2	2.18	0.77
91:4N:101:PGV:H12	91:4N:101:PGV:H161	1.67	0.77
24:1Y:75:ILE:HG23	69:1Y:201:3PE:C27	2.11	0.77
31:1f:11:TRP:CZ3	69:1f:101:3PE:H362	2.20	0.77
75:3N:502:CDL:H592	69:3P:511:3PE:H2G2	1.67	0.77
46:3O:197:ASN:HB3	46:3O:232:LEU:HB2	1.65	0.77
57:4C:55:TYR:HA	75:4C:307:CDL:H782	1.67	0.77
69:1Y:209:3PE:H3C2	69:1Y:212:3PE:H2E1	1.65	0.77
38:1m:99:PHE:HE2	69:1m:205:3PE:H3G2	1.44	0.77
69:1m:202:3PE:H271	69:1m:202:3PE:H222	1.64	0.77
47:3C:267:HIS:CE1	47:3C:269:LYS:HB3	2.20	0.77
48:3Q:144:ARG:HE	48:3Q:147:LEU:HD13	1.47	0.77
69:3J:105:3PE:H2G1	69:3Y:102:3PE:H391	1.66	0.77
69:3R:305:3PE:H12	51:3T:25:ALA:H	1.49	0.77
56:4B:39:LEU:HD22	75:4B:302:CDL:H432	1.67	0.77
75:3P:513:CDL:H231	69:3P:520:3PE:H2F2	1.66	0.76
69:3Y:101:3PE:H2H2	69:3Y:104:3PE:H3E1	1.67	0.76
2:1B:177:TYR:HA	70:1B:202:PC1:C27	2.14	0.76
12:1L:534:HIS:CB	69:1L:701:3PE:H31	2.16	0.76
69:1L:712:3PE:H262	69:1L:712:3PE:H321	1.65	0.76
4:1D:52:GLY:H	4:1D:53:PRO:HD3	1.49	0.76
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.17	0.76
14:1N:8:THR:HG22	75:1N:402:CDL:C41	2.15	0.76
69:1Y:208:3PE:H3I1	69:1Y:211:3PE:H332	1.65	0.76
69:1Y:215:3PE:H331	69:1Y:216:3PE:H371	1.66	0.76
31:1f:45:LYS:O	41:1p:68:ARG:NH2	2.18	0.76
45:3A:91:THR:HG22	45:3A:94:HIS:H	1.50	0.76
47:3P:342:PRO:HB2	47:3P:344:GLU:HG2	1.65	0.76
69:3P:506:3PE:H351	69:3P:506:3PE:H281	1.67	0.76
7:1G:226:GLU:HG2	7:1G:253:ARG:HD3	1.67	0.76
12:1L:161:ARG:HG2	12:1L:164:ALA:H	1.49	0.76
75:1d:205:CDL:H351	75:1d:205:CDL:H122	1.66	0.76
37:1l:111:PHE:CE2	69:1l:203:3PE:C28	2.63	0.76
75:1q:202:CDL:H132	75:1q:202:CDL:HA61	1.67	0.76
69:1M:502:3PE:H351	69:1M:502:3PE:H2B1	1.68	0.76
75:3A:501:CDL:H241	75:3A:501:CDL:H451	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3S:201:3PE:H2C2	70:3T:102:PC1:H291	1.66	0.76
69:3W:103:3PE:H291	69:3W:103:3PE:H112	1.66	0.76
15:1O:133:VAL:HG21	15:1O:206:TYR:CD2	2.21	0.76
47:3C:286:ASN:HB2	69:3C:512:3PE:H2	1.65	0.76
69:3C:517:3PE:H12	69:4G:101:3PE:H112	1.66	0.76
69:3G:104:3PE:H352	69:3G:104:3PE:H252	1.68	0.76
69:3N:501:3PE:H3B1	47:3P:14:ILE:HD11	1.68	0.76
47:3P:306:MET:HE2	69:3P:514:3PE:H241	1.65	0.76
24:1Y:27:ILE:HD12	69:1Y:208:3PE:H3F1	1.68	0.76
32:1g:59:ARG:HH22	69:1g:203:3PE:H11	1.49	0.76
69:3P:507:3PE:C21	69:3P:507:3PE:H321	2.16	0.76
69:3P:507:3PE:H222	54:3Y:38:TRP:CD1	2.21	0.76
75:4C:307:CDL:H152	75:4C:307:CDL:HB22	1.66	0.76
9:1I:45:PRO:CD	26:1a:1:MET:HG3	2.16	0.76
69:1Z:201:3PE:H331	69:1Z:201:3PE:H2C1	1.66	0.76
48:3D:313:ARG:HD3	51:3G:28:PHE:CE2	2.21	0.76
69:3Q:504:3PE:H2	69:3Q:504:3PE:H231	1.68	0.76
69:3Y:104:3PE:H272	69:3Y:104:3PE:H2B1	1.66	0.76
75:4C:306:CDL:HB4	75:4C:306:CDL:H131	1.66	0.76
24:1Y:5:LEU:CD2	69:1Y:211:3PE:O32	2.34	0.76
70:1Y:207:PC1:H281	69:1Y:209:3PE:H391	1.67	0.76
70:1d:204:PC1:H232	70:1d:204:PC1:P	2.26	0.76
47:3C:289:GLY:C	69:3C:512:3PE:H351	2.11	0.76
7:1G:203:CYS:SG	71:1G:802:SF4:FE4	1.77	0.76
70:1H:403:PC1:H252	10:1J:45:LEU:CB	2.16	0.76
57:4C:137:LEU:HD13	57:4C:246:ASP:HA	1.68	0.76
91:4C:304:PGV:H131	91:4C:304:PGV:H321	1.68	0.76
75:4C:306:CDL:H322	75:4C:306:CDL:H182	1.68	0.76
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.68	0.75
75:1g:201:CDL:H331	75:1g:201:CDL:H142	1.66	0.75
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.67	0.75
47:3C:4:ILE:HG12	47:3C:8:HIS:HB2	1.69	0.75
47:3C:359:PHE:CG	69:3C:511:3PE:H3C1	2.20	0.75
75:1d:202:CDL:H542	75:1d:202:CDL:H341	1.66	0.75
37:1l:106:SER:HB2	69:1l:202:3PE:H352	1.68	0.75
5:1E:149:VAL:HG21	6:1F:267:THR:HG22	1.65	0.75
12:1L:602:PHE:CZ	69:1L:706:3PE:H332	2.21	0.75
69:1Y:214:3PE:H3A2	69:1Y:214:3PE:H341	1.67	0.75
69:1Y:215:3PE:H3C2	70:3T:102:PC1:H3C2	1.68	0.75
27:1b:27:LEU:CD1	69:1b:101:3PE:H2G1	2.16	0.75
69:3N:501:3PE:H392	69:3P:511:3PE:H3B2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1Z:201:3PE:H12	69:1Z:201:3PE:H112	1.68	0.75
69:3R:305:3PE:H2D2	69:3R:305:3PE:H2H2	1.68	0.75
55:4A:222:PRO:HG2	56:4B:176:PRO:HB2	1.69	0.75
56:4B:61:VAL:HG11	93:4B:303:PSC:C4	2.16	0.75
20:1T:70:LEU:HD23	20:1T:76:ILE:HG13	1.68	0.75
47:3C:154:PRO:O	69:3C:509:3PE:H2B2	1.86	0.75
47:3C:283:SER:OG	69:3C:511:3PE:H371	1.86	0.75
46:3B:51:ILE:HG12	46:3B:204:MET:HG2	1.68	0.75
69:1d:206:3PE:C38	69:1f:104:3PE:H2A2	2.15	0.75
32:1g:63:PHE:HE2	75:1g:201:CDL:H221	1.50	0.75
47:3C:379:TRP:CE3	50:3F:45:ARG:HD3	2.22	0.75
69:3P:516:3PE:H3B1	70:3T:102:PC1:H2A2	1.66	0.75
49:3R:224:PRO:HB3	49:3R:243:TYR:HE2	1.51	0.75
55:4A:109:PHE:CB	91:4A:609:PGV:H171	2.06	0.75
75:1Y:217:CDL:H212	69:3S:201:3PE:H3C2	1.68	0.75
24:1Y:62:SER:O	69:1Y:208:3PE:H382	1.87	0.75
49:3R:235:TYR:HB2	49:3R:242:HIS:HB3	1.66	0.75
32:1g:59:ARG:NH2	69:1g:203:3PE:H11	2.02	0.74
40:1o:56:ASP:OD1	40:1o:57:TYR:N	2.18	0.74
45:3A:242:ARG:HB2	51:3G:17:THR:CG2	2.17	0.74
25:1Z:29:GLY:H	69:1Z:201:3PE:H111	1.50	0.74
45:3A:39:VAL:HG11	45:3A:195:MET:HE3	1.69	0.74
51:3T:72:LYS:HD2	52:3U:52:GLU:HG3	1.68	0.74
70:3T:102:PC1:H322	70:3T:102:PC1:H232	1.69	0.74
69:3X:105:3PE:H352	69:3X:105:3PE:H232	1.69	0.74
70:1H:403:PC1:H271	10:1J:45:LEU:HD12	1.69	0.74
47:3C:278:TYR:CZ	47:3C:282:ARG:HD3	2.23	0.74
46:3O:35:ILE:HD13	46:3O:206:LEU:HB3	1.68	0.74
47:3P:287:LYS:HB2	69:3P:503:3PE:H122	1.69	0.74
48:3Q:144:ARG:HG3	48:3Q:147:LEU:HB2	1.68	0.74
69:3W:103:3PE:H111	69:3W:103:3PE:O32	1.88	0.74
75:1H:401:CDL:H122	16:1P:189:GLY:H	1.50	0.74
75:1i:201:CDL:H562	41:1p:44:VAL:HG12	1.70	0.74
39:1n:55:ASP:OD1	45:3N:221:GLY:O	2.04	0.74
24:1Y:62:SER:CA	69:1Y:208:3PE:H371	2.17	0.74
24:1Y:87:LEU:HD11	69:1Y:212:3PE:H351	1.68	0.74
29:1d:27:THR:HB	69:1f:104:3PE:H261	1.69	0.74
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.20	0.74
69:3C:506:3PE:H232	69:3C:507:3PE:H11	1.70	0.74
69:3C:516:3PE:H3A1	69:3C:516:3PE:H2D1	1.68	0.74
91:4A:609:PGV:H252	66:4L:28:TYR:HB2	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:345:SER:OG	70:1d:204:PC1:H392	1.88	0.74
15:1O:77:CYS:HB2	15:1O:96:LEU:HB2	1.69	0.74
69:3C:515:3PE:H391	69:3C:515:3PE:H342	1.69	0.74
75:1d:202:CDL:H273	75:1d:202:CDL:H342	1.70	0.74
75:1q:202:CDL:H252	75:1q:202:CDL:H421	1.69	0.74
49:3E:212:ILE:HG22	49:3E:261:PRO:HG2	1.68	0.74
49:3E:249:ILE:H	49:3E:257:ASN:HB3	1.52	0.74
33:1h:78:THR:O	70:1h:203:PC1:C15	2.35	0.74
38:1m:92:PHE:CZ	69:1m:203:3PE:H252	2.23	0.74
45:3N:14:THR:HG21	45:3N:389:ARG:CB	2.17	0.74
54:3Y:23:MET:CE	69:3Y:101:3PE:H342	2.17	0.74
91:4A:609:PGV:C20	66:4L:28:TYR:CE1	2.70	0.74
69:1L:709:3PE:H321	69:1L:709:3PE:H251	1.69	0.74
69:3C:509:3PE:H341	69:3C:509:3PE:H242	1.67	0.74
54:3Y:5:PHE:CE1	75:3Y:106:CDL:H312	2.22	0.74
4:1D:34:ASN:HB2	15:1O:158:VAL:HG13	1.68	0.74
49:3E:169:TRP:CE2	49:3E:273:VAL:HG12	2.23	0.74
69:3P:506:3PE:H3I2	69:3P:517:3PE:H371	1.70	0.74
12:1L:512:LYS:HG2	64:4J:16:ASN:HD22	1.53	0.73
16:1P:270:PHE:CD2	16:1P:278:TRP:HB2	2.23	0.73
91:4A:608:PGV:H343	75:4B:302:CDL:H872	1.70	0.73
91:4A:608:PGV:C34	75:4B:302:CDL:C87	2.65	0.73
24:1Y:75:ILE:HG21	69:1Y:201:3PE:C28	2.18	0.73
75:1d:202:CDL:H1	31:1f:33:LYS:HE2	1.69	0.73
49:3R:179:ARG:HH21	49:3R:184:ILE:HA	1.53	0.73
12:1L:464:ALA:HB2	69:1L:703:3PE:H2A2	1.68	0.73
69:1N:401:3PE:H2E1	69:1d:201:3PE:H2G1	1.68	0.73
29:1d:29:PRO:HG3	75:1d:202:CDL:HB4	1.69	0.73
45:3N:30:SER:HB2	45:3N:32:GLN:HG3	1.70	0.73
75:3P:513:CDL:H202	69:3P:520:3PE:H2D1	1.71	0.73
56:4B:61:VAL:HG11	93:4B:303:PSC:C5	2.17	0.73
62:4H:25:GLN:HE21	62:4H:28:ASN:HD22	1.35	0.73
12:1L:149:ILE:HG21	75:1L:704:CDL:H752	1.68	0.73
48:3Q:140:GLY:HA3	52:3U:53:ASP:HA	1.69	0.73
75:4B:302:CDL:H372	75:4B:302:CDL:H141	1.71	0.73
57:4C:12:ASN:HD21	64:4J:20:VAL:HG23	1.54	0.73
1:1A:36:PRO:HB2	1:1A:43:PRO:HG2	1.69	0.73
8:1H:138:GLN:NE2	8:1H:194:ASN:OD1	2.22	0.73
24:1Y:31:THR:OG1	69:1Y:208:3PE:H2E1	1.89	0.73
46:3B:95:LYS:HD3	46:3B:96:LEU:N	2.04	0.73
69:3W:102:3PE:H361	69:3X:101:3PE:H342	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:28:TYR:OH	69:1B:205:3PE:O12	2.07	0.73
12:1L:566:THR:O	12:1L:570:GLN:HG2	1.89	0.73
46:3B:166:ALA:HB2	46:3B:244:ILE:HG13	1.71	0.73
69:3C:506:3PE:H271	69:3C:507:3PE:H321	1.70	0.73
69:3N:501:3PE:H2A1	75:3N:502:CDL:H532	1.70	0.73
69:3P:507:3PE:H291	69:3P:507:3PE:H3A2	1.68	0.73
75:3P:513:CDL:H412	69:3P:519:3PE:H2A2	1.69	0.73
10:1J:87:LYS:CB	69:1J:201:3PE:O14	2.37	0.73
24:1Y:109:ILE:HG12	70:1Y:206:PC1:H321	1.71	0.73
75:3F:201:CDL:H802	75:3F:201:CDL:H842	1.70	0.73
75:3N:502:CDL:H311	47:3P:19:ILE:HG12	1.71	0.73
46:3O:169:ARG:HG3	46:3O:240:ARG:HB3	1.70	0.73
8:1H:196:ALA:HB3	8:1H:197:PRO:HD3	1.71	0.73
24:1Y:31:THR:O	24:1Y:35:VAL:HG12	1.89	0.73
69:1Y:215:3PE:H31	69:3P:510:3PE:H221	1.71	0.73
47:3C:95:PHE:CD1	69:3C:503:3PE:H3D1	2.24	0.73
45:3N:68:LYS:HG2	45:3N:119:ASN:HB3	1.70	0.73
49:3R:153:GLU:HG3	49:3R:169:TRP:CD2	2.24	0.73
91:4A:609:PGV:O03	66:4L:28:TYR:OH	2.06	0.73
7:1G:55:CYS:SG	72:1G:803:FES:FE2	1.79	0.73
69:3J:104:3PE:H3D2	69:3J:104:3PE:H2D2	1.69	0.73
49:3R:225:ILE:HG13	49:3R:235:TYR:CE2	2.23	0.73
75:1L:704:CDL:H571	13:1M:369:LEU:HB3	1.71	0.73
32:1g:56:TRP:CZ3	69:1g:202:3PE:H361	2.24	0.73
69:3G:104:3PE:H251	69:3G:105:3PE:H351	1.68	0.73
75:3N:502:CDL:H572	75:3N:502:CDL:H182	1.71	0.73
49:3R:263:TYR:HA	49:3R:273:VAL:HA	1.70	0.73
2:1B:176:TRP:CZ3	70:1B:202:PC1:H231	2.17	0.72
37:1l:106:SER:OG	69:1l:203:3PE:H341	1.88	0.72
69:3C:507:3PE:H3G2	69:3C:511:3PE:H2B2	1.69	0.72
75:3F:201:CDL:H181	69:3G:109:3PE:H231	1.71	0.72
69:3W:101:3PE:H272	69:3W:102:3PE:H221	1.69	0.72
69:3X:107:3PE:H252	69:3X:107:3PE:O21	1.89	0.72
1:1A:23:TRP:HE3	70:1P:502:PC1:H242	1.53	0.72
1:1A:108:GLN:NE2	69:1A:203:3PE:C25	2.50	0.72
13:1M:19:LYS:NZ	31:1f:9:ASP:OD2	2.20	0.72
47:3C:377:LEU:HG	50:3F:32:TYR:HE2	1.52	0.72
57:4C:179:SER:HB3	91:4C:304:PGV:H012	1.69	0.72
70:1B:203:PC1:H291	75:1q:202:CDL:H631	1.71	0.72
14:1N:256:PRO:HG2	69:1N:401:3PE:H2F2	1.72	0.72
69:3C:517:3PE:H242	69:3C:517:3PE:H282	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:173:ASN:HA	45:3N:176:LYS:HG2	1.70	0.72
69:4G:104:3PE:H121	69:4G:104:3PE:H222	1.71	0.72
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.71	0.72
70:1M:501:PC1:O22	75:1i:201:CDL:H162	1.90	0.72
24:1Y:75:ILE:HG22	69:1Y:214:3PE:C26	2.16	0.72
31:1f:21:VAL:CG1	69:1f:103:3PE:H361	2.20	0.72
69:3C:513:3PE:H331	69:3X:107:3PE:H262	1.70	0.72
51:3G:33:THR:HA	69:3G:103:3PE:H221	1.71	0.72
69:3G:106:3PE:H222	69:3G:106:3PE:H322	1.72	0.72
54:3Y:44:TRP:CD1	69:3Y:105:3PE:H381	2.24	0.72
13:1M:8:THR:O	13:1M:11:LEU:HB2	1.89	0.72
20:1T:25:ILE:HD11	20:1T:42:LEU:HD11	1.71	0.72
34:1i:88:HIS:CE1	75:1i:201:CDL:OB3	2.43	0.72
38:1m:87:LEU:HB3	69:1m:202:3PE:H251	1.71	0.72
47:3C:124:MET:HE1	47:3C:298:ILE:HD13	1.72	0.72
69:3C:515:3PE:H2I1	69:3C:516:3PE:H2F1	1.70	0.72
75:1Y:217:CDL:H562	75:1Y:217:CDL:H832	1.70	0.72
49:3E:150:SER:HB3	49:3E:170:ARG:HG3	1.72	0.72
69:3J:104:3PE:H2H2	69:3J:104:3PE:H3H1	1.71	0.72
47:3P:356:ILE:HG23	69:3P:506:3PE:H3I1	1.71	0.72
54:3X:18:ILE:HG12	75:3X:103:CDL:H212	1.71	0.72
9:1I:148:LEU:HD23	17:1Q:70:MET:HG3	1.72	0.72
12:1L:504:LEU:CD1	69:1L:707:3PE:N	2.53	0.72
43:1r:72:GLN:N	43:1r:72:GLN:OE1	2.22	0.72
48:3D:299:MET:HA	69:3D:502:3PE:H2B1	1.71	0.72
49:3E:125:VAL:HG21	70:3J:106:PC1:H362	1.72	0.72
69:3P:511:3PE:H3A1	69:3P:512:3PE:C39	2.19	0.72
55:4A:381:LEU:HD13	88:4A:601:HEA:HAC	1.71	0.72
69:1L:709:3PE:H3A2	75:1i:201:CDL:H771	1.72	0.72
75:1g:201:CDL:HA21	33:1h:24:LEU:CD1	2.18	0.72
13:1M:127:VAL:CG1	69:1N:401:3PE:H3F2	2.19	0.72
14:1N:277:ILE:HG13	82:1Y:203:PGT:H161	1.71	0.72
16:1P:194:ILE:HD12	16:1P:288:HIS:HD2	1.55	0.72
31:1f:17:PRO:HB3	69:1f:102:3PE:H2G2	1.71	0.72
69:3C:510:3PE:C12	69:3C:510:3PE:C1	2.49	0.72
49:3E:264:GLU:H	49:3E:272:ILE:HG12	1.53	0.72
56:4B:35:SER:HB3	75:4B:302:CDL:H402	1.69	0.72
69:1m:202:3PE:H291	69:1m:203:3PE:H322	1.69	0.72
75:1L:704:CDL:H581	13:1M:372:SER:HB3	1.72	0.71
69:1Y:215:3PE:H2B1	69:1Y:216:3PE:H262	1.72	0.71
69:1d:206:3PE:H372	69:1f:104:3PE:H2B1	1.67	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:106:SER:HB2	69:1l:202:3PE:C35	2.20	0.71
38:1m:92:PHE:CE1	69:1m:203:3PE:H362	2.25	0.71
49:3E:155:LYS:HE2	49:3E:274:GLY:OXT	1.89	0.71
69:3P:503:3PE:H2A1	69:3P:505:3PE:H361	1.72	0.71
69:3P:518:3PE:H352	69:3P:518:3PE:H2A2	1.72	0.71
16:1P:52:GLU:HG3	16:1P:54:TYR:H	1.54	0.71
45:3A:91:THR:HG23	45:3A:93:GLU:H	1.54	0.71
47:3C:376:LEU:O	50:3F:29:ARG:HD3	1.90	0.71
49:3E:151:LYS:HG2	49:3E:152:ILE:HG23	1.72	0.71
45:3N:240:GLU:HG3	45:3N:422:VAL:HB	1.70	0.71
2:1B:176:TRP:O	70:1B:202:PC1:C25	2.36	0.71
12:1L:78:LEU:HD22	69:1L:702:3PE:H371	1.72	0.71
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.72	0.71
75:1g:201:CDL:H311	33:1h:31:LEU:HD21	1.72	0.71
39:1n:97:LYS:HG2	39:1n:177:PRO:HG3	1.72	0.71
69:3C:511:3PE:H3A2	69:3C:512:3PE:H2D2	1.71	0.71
69:3N:501:3PE:H382	75:3N:502:CDL:H161	1.72	0.71
69:1d:201:3PE:H372	69:1d:201:3PE:H252	1.72	0.71
69:3A:502:3PE:H362	69:3A:502:3PE:H262	1.71	0.71
46:3O:128:ALA:HA	46:3O:227:ARG:HH22	1.55	0.71
91:4A:609:PGV:C20	66:4L:28:TYR:CZ	2.74	0.71
91:4C:303:PGV:H72	91:4C:303:PGV:H272	1.72	0.71
8:1H:179:TRP:CD2	8:1H:180:PRO:HD3	2.25	0.71
20:1U:8:LEU:HD11	34:1i:19:ARG:HH21	1.55	0.71
69:1m:203:3PE:H262	69:1m:203:3PE:H2B2	1.73	0.71
46:3B:56:ARG:HD2	46:3B:103:GLU:HG2	1.71	0.71
49:3E:155:LYS:HD3	49:3E:176:VAL:HG21	1.72	0.71
69:3G:111:3PE:H292	69:3G:111:3PE:H231	1.71	0.71
69:3P:510:3PE:H2I3	51:3T:54:VAL:HG21	1.73	0.71
49:3R:195:LEU:HB3	49:3R:248:ARG:HH21	1.55	0.71
40:1o:77:LEU:HD12	69:1o:201:3PE:H261	1.69	0.71
45:3A:19:LEU:HD22	45:3A:213:GLN:HG2	1.73	0.71
45:3A:188:GLN:HG3	45:3A:189:HIS:CD2	2.26	0.71
69:3A:502:3PE:H3B1	69:3A:502:3PE:H3F2	1.72	0.71
50:3F:119:TRP:CZ2	46:3O:87:ARG:HB3	2.26	0.71
47:3P:249:LEU:CD1	69:3P:520:3PE:H221	2.20	0.71
69:3P:508:3PE:H2G1	69:3P:519:3PE:H3G2	1.73	0.71
49:3R:150:SER:O	49:3R:151:LYS:C	2.33	0.71
91:4C:303:PGV:H201	68:4N:36:LEU:HB3	1.72	0.71
45:3A:131:ARG:HD3	45:3A:175:ARG:HA	1.71	0.71
69:3P:510:3PE:H32	69:3P:510:3PE:H122	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:289:ALA:C	55:4A:291:HIS:H	1.98	0.71
4:1D:34:ASN:HB3	4:1D:36:VAL:HG22	1.72	0.71
32:1g:59:ARG:HB3	75:1g:201:CDL:H161	1.71	0.71
49:3E:223:VAL:HG11	48:3Q:106:ASN:O	1.90	0.71
47:3P:320:LEU:HD23	70:3T:102:PC1:H242	1.71	0.71
49:3R:155:LYS:HE2	49:3R:271:VAL:HG23	1.72	0.71
54:3Y:41:ILE:CD1	69:3Y:105:3PE:H291	2.20	0.71
57:4C:151:LEU:HD22	57:4C:159:MET:HE3	1.73	0.71
58:4D:51:LEU:O	58:4D:56:LYS:NZ	2.22	0.71
1:1A:57:LEU:HD21	10:1J:172:THR:HG21	1.73	0.71
2:1B:176:TRP:CH2	70:1B:202:PC1:H241	2.25	0.71
6:1F:91:LYS:HB2	6:1F:131:ALA:HA	1.73	0.71
14:1N:129:LEU:HD13	75:1N:402:CDL:H542	1.73	0.71
24:1Y:75:ILE:HG21	69:1Y:201:3PE:H271	1.68	0.71
27:1b:23:ALA:HB1	69:1b:101:3PE:H2G2	1.71	0.71
33:1h:78:THR:HG21	69:1h:204:3PE:H282	1.73	0.71
75:3A:501:CDL:H111	69:3A:503:3PE:H342	1.72	0.71
49:3E:244:ASP:HB2	49:3E:250:ARG:HG2	1.71	0.71
54:3Y:41:ILE:CD1	69:3Y:105:3PE:C37	2.69	0.71
91:4A:609:PGV:C26	66:4L:28:TYR:HB3	2.21	0.71
57:4C:43:LEU:HD21	91:4G:102:PGV:H282	1.73	0.71
69:1B:204:3PE:H2I2	69:1B:205:3PE:H2I2	1.71	0.71
13:1M:127:VAL:HG11	69:1N:401:3PE:C3G	2.21	0.71
14:1N:276:ILE:HG21	82:1Y:203:PGT:O3	1.90	0.71
47:3C:289:GLY:HA3	69:3C:512:3PE:H332	1.71	0.71
69:3P:511:3PE:H2G1	69:3P:511:3PE:H371	1.72	0.71
54:3X:5:PHE:CE2	69:3X:105:3PE:H221	2.25	0.71
91:4C:302:PGV:C29	75:4C:307:CDL:C40	2.63	0.71
8:1H:32:GLN:OE1	8:1H:34:ARG:NH1	2.24	0.70
10:1J:23:LYS:HB2	11:1K:23:ARG:HD2	1.73	0.70
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.25	0.70
69:1N:401:3PE:H2E1	69:1d:201:3PE:H2I2	1.73	0.70
24:1Y:107:TYR:CE1	69:1Y:209:3PE:H31	2.25	0.70
69:1Y:205:3PE:H262	69:1Y:208:3PE:H351	1.71	0.70
25:1Z:78:GLU:OE1	26:1a:50:ARG:NH1	2.24	0.70
70:1d:204:PC1:H232	70:1d:204:PC1:O14	1.91	0.70
46:3B:37:SER:HB3	46:3B:216:LEU:HD12	1.73	0.70
69:3C:509:3PE:H3H1	75:3N:502:CDL:H871	1.71	0.70
49:3E:186:GLN:O	49:3E:190:VAL:HG23	1.91	0.70
49:3R:213:LEU:HD22	49:3R:258:LEU:HB2	1.72	0.70
32:1g:68:ILE:CD1	75:1g:201:CDL:H261	2.14	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1k:101:3PE:H391	69:1k:101:3PE:H271	1.71	0.70
45:3A:349:ALA:O	45:3A:350:THR:HB	1.89	0.70
47:3C:155:TYR:HB3	69:3C:509:3PE:H2A2	1.71	0.70
49:3R:179:ARG:HH11	49:3R:211:VAL:HB	1.55	0.70
69:3W:101:3PE:H3I1	69:3W:102:3PE:H3D2	1.72	0.70
91:4A:609:PGV:C20	66:4L:28:TYR:CE2	2.72	0.70
5:1E:86:PHE:O	7:1G:177:ARG:HD3	1.91	0.70
14:1N:29:ILE:HG13	14:1N:86:ILE:HD11	1.73	0.70
32:1g:56:TRP:CZ2	69:1g:202:3PE:H342	2.26	0.70
49:3R:187:GLU:HG2	49:3R:245:ALA:HB3	1.73	0.70
14:1N:162:ILE:HD13	14:1N:282:MET:HB3	1.73	0.70
45:3A:91:THR:CG2	45:3A:94:HIS:H	2.04	0.70
47:3C:32:ASN:HD21	47:3C:227:LYS:HE2	1.57	0.70
47:3C:360:LEU:HA	69:3C:512:3PE:C2I	2.19	0.70
47:3P:377:LEU:HG	50:3S:20:TYR:HE2	1.57	0.70
69:3P:506:3PE:H362	69:3P:506:3PE:H2A2	1.73	0.70
70:1B:203:PC1:H2A1	8:1H:46:LEU:HD21	1.71	0.70
76:1I:203:AYA:HB1	42:1q:54:GLN:CD	2.15	0.70
24:1Y:108:GLY:HA3	70:1Y:206:PC1:H232	1.70	0.70
29:1d:27:THR:HG23	69:1d:206:3PE:O12	1.92	0.70
75:1d:205:CDL:H782	75:1d:205:CDL:H271	1.72	0.70
48:3Q:240:PRO:HD3	51:3T:12:HIS:CD2	2.27	0.70
69:3X:105:3PE:H112	69:3X:105:3PE:H222	1.74	0.70
54:3Y:41:ILE:HD13	69:3Y:105:3PE:C37	2.17	0.70
55:4A:21:LEU:HD13	91:4A:609:PGV:H62	1.72	0.70
75:1H:401:CDL:H122	16:1P:189:GLY:N	2.06	0.70
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.72	0.70
16:1P:275:PHE:O	16:1P:276:GLU:C	2.32	0.70
23:1X:87:CYS:SG	23:1X:102:GLN:NE2	2.65	0.70
24:1Y:112:ALA:HA	70:1Y:206:PC1:H292	1.72	0.70
69:1f:101:3PE:H2A1	69:1f:101:3PE:H372	1.73	0.70
75:3A:501:CDL:H541	69:3C:516:3PE:H3B2	1.74	0.70
46:3B:35:ILE:HD11	46:3B:220:ALA:HB2	1.74	0.70
48:3D:115:ARG:HB2	48:3D:143:CYS:HB2	1.73	0.70
70:3R:303:PC1:H2G1	70:3X:104:PC1:H2I2	1.74	0.70
87:3X:102:PEK:H242	87:3X:102:PEK:H292	1.74	0.70
2:1B:177:TYR:CA	70:1B:202:PC1:C26	2.66	0.70
31:1f:10:HIS:HE1	69:1f:102:3PE:O22	1.72	0.70
47:3P:108:MET:HA	47:3P:108:MET:HE2	1.73	0.70
2:1B:91:THR:HG23	2:1B:119:CYS:HB3	1.73	0.70
14:1N:142:LEU:HB3	14:1N:194:LEU:HD21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	1.99	0.70
69:1Y:201:3PE:H331	51:3T:56:TYR:HD1	1.55	0.70
46:3B:227:ARG:HD3	46:3B:231:GLY:H	1.56	0.70
69:3J:105:3PE:C2G	69:3Y:102:3PE:H3B1	2.22	0.70
55:4A:86:MET:HE1	55:4A:184:PHE:HB3	1.73	0.70
5:1E:87:TYR:CD1	6:1F:181:ALA:HB3	2.27	0.70
12:1L:463:PHE:CZ	69:1k:101:3PE:H3G2	2.27	0.70
27:1b:27:LEU:CD1	69:1b:101:3PE:C2F	2.69	0.70
49:3R:243:TYR:HB3	49:3R:247:GLY:HA2	1.73	0.70
2:1B:42:ARG:CZ	70:1B:203:PC1:O12	2.39	0.70
43:1r:11:ARG:HD3	43:1r:19:LEU:HD11	1.72	0.70
49:3E:179:ARG:HG3	49:3E:211:VAL:H	1.57	0.70
50:3F:25:LEU:HD13	50:3F:28:ILE:HB	1.73	0.70
93:4B:303:PSC:H211	63:4I:17:LEU:HD23	1.74	0.70
2:1B:177:TYR:CA	70:1B:202:PC1:H261	2.21	0.69
49:3E:155:LYS:CD	49:3E:274:GLY:OXT	2.40	0.69
47:3P:315:MET:HE1	47:3P:325:PHE:HB2	1.74	0.69
6:1F:361:GLN:HE22	17:1Q:133:LYS:HZ3	1.37	0.69
9:1I:68:ARG:HD2	9:1I:132:VAL:HG11	1.74	0.69
69:1L:709:3PE:C37	75:1i:201:CDL:H781	2.21	0.69
45:3N:195:MET:SD	45:3N:219:LEU:HD11	2.32	0.69
47:3P:10:LEU:CD2	69:3P:512:3PE:H381	2.15	0.69
69:3P:503:3PE:H382	69:3P:505:3PE:H352	1.75	0.69
48:3Q:156:GLN:HG2	52:3U:59:PHE:HZ	1.55	0.69
49:3R:179:ARG:NH2	49:3R:184:ILE:HA	2.08	0.69
4:1D:165:THR:OG1	8:1H:275:ALA:O	2.11	0.69
24:1Y:62:SER:O	69:1Y:208:3PE:C38	2.40	0.69
69:1g:202:3PE:H31	69:1g:202:3PE:N	2.07	0.69
38:1m:91:LEU:CD1	69:1m:202:3PE:H281	2.21	0.69
47:3C:237:LEU:HD13	48:3D:301:MET:HG3	1.74	0.69
69:3J:105:3PE:H2E1	69:3Y:102:3PE:C39	2.22	0.69
46:3O:166:ALA:HB2	46:3O:244:ILE:HG13	1.74	0.69
47:3P:92:ILE:HD13	69:3P:519:3PE:H2B1	1.74	0.69
2:1B:175:ILE:HD13	2:1B:178:ARG:HH11	1.56	0.69
31:1f:25:TYR:HE1	69:1f:104:3PE:H221	1.56	0.69
69:3C:513:3PE:H241	69:3C:517:3PE:C35	2.21	0.69
55:4A:408:ALA:HB3	91:4A:606:PGV:H21	1.75	0.69
75:4B:302:CDL:OA9	63:4I:35:TYR:HE1	1.76	0.69
68:4N:2:LEU:H	68:4N:2:LEU:CD1	2.05	0.69
2:1B:150:PRO:HG3	4:1D:189:MET:HE2	1.72	0.69
22:1W:31:ARG:HA	22:1W:34:GLU:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1d:206:3PE:H372	69:1f:104:3PE:C2B	2.22	0.69
47:3C:141:TRP:HB3	47:3C:268:ILE:HD13	1.74	0.69
49:3E:159:ILE:H	49:3E:159:ILE:HD12	1.58	0.69
69:3P:507:3PE:C22	54:3Y:38:TRP:CD1	2.75	0.69
5:1E:151:ALA:O	5:1E:152:PRO:C	2.34	0.69
12:1L:29:THR:HG23	12:1L:31:LEU:H	1.58	0.69
24:1Y:27:ILE:HB	69:1Y:208:3PE:C3D	2.16	0.69
27:1b:27:LEU:HD12	69:1b:101:3PE:H2D1	0.82	0.69
34:1i:38:ARG:HH21	34:1i:40:TRP:HA	1.58	0.69
69:1Y:209:3PE:H3B2	75:3P:513:CDL:H852	1.73	0.69
29:1d:8:ARG:HG2	70:1d:204:PC1:C24	2.22	0.69
48:3Q:3:LEU:HD21	52:3U:56:GLU:CD	2.17	0.69
49:3R:179:ARG:HE	49:3R:184:ILE:HG12	1.58	0.69
2:1B:25:ARG:HG2	2:1B:27:GLU:H	1.58	0.69
12:1L:592:LEU:HG	12:1L:596:MET:HE2	1.75	0.69
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	1.75	0.69
24:1Y:4:LEU:HD21	24:1Y:27:ILE:HA	1.74	0.69
24:1Y:105:ARG:NH1	70:1Y:207:PC1:O12	2.25	0.69
24:1Y:109:ILE:HA	70:1Y:206:PC1:H332	1.73	0.69
31:1f:14:ILE:HD13	69:1f:101:3PE:H2B2	1.73	0.69
38:1m:7:PRO:HB3	38:1m:13:LEU:HB2	1.75	0.69
46:3B:71:LEU:HD23	49:3I:68:VAL:HG11	1.75	0.69
49:3E:263:TYR:HB3	49:3E:273:VAL:HG22	1.74	0.69
45:3N:86:LEU:HB3	46:3O:285:VAL:HG22	1.75	0.69
48:3Q:224:ARG:HD3	51:3T:26:PHE:CE2	2.28	0.69
69:3Q:503:3PE:H361	69:3W:101:3PE:H341	1.75	0.69
69:1L:701:3PE:H332	69:1L:701:3PE:H32	1.75	0.69
23:1X:19:VAL:O	26:1a:50:ARG:NH2	2.26	0.69
24:1Y:86:PRO:C	70:1Y:202:PC1:H341	2.18	0.69
31:1f:22:PHE:CE2	69:1f:104:3PE:H372	2.27	0.69
47:3C:46:LEU:HD21	69:3E:303:3PE:H2D1	1.75	0.69
48:3D:195:GLY:HA3	49:3R:223:VAL:HG21	1.75	0.69
69:3J:101:3PE:H2C1	69:3J:101:3PE:H391	1.75	0.69
49:3R:162:GLY:N	49:3R:178:HIS:HB3	2.08	0.69
69:3W:102:3PE:H322	69:3X:101:3PE:H332	1.74	0.69
65:4K:34:THR:HG21	91:4K:101:PGV:H202	1.75	0.69
2:1B:92:LEU:O	2:1B:133:VAL:HG12	1.93	0.69
2:1B:175:ILE:HD13	2:1B:178:ARG:NH1	2.08	0.69
7:1G:122:MET:HA	43:1r:60:ARG:HH22	1.56	0.69
14:1N:133:TRP:HE3	75:1N:402:CDL:H591	1.58	0.69
29:1d:33:TYR:CD1	75:1d:202:CDL:H411	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:305:GLN:NE2	49:3I:42:VAL:HG12	2.08	0.69
69:3C:509:3PE:H241	69:3X:107:3PE:H372	1.75	0.69
69:3C:516:3PE:O12	75:3Y:106:CDL:H521	1.93	0.69
53:3J:46:HIS:HD2	69:3J:101:3PE:H342	1.56	0.69
17:1Q:43:ASN:OD1	17:1Q:45:MET:HB2	1.93	0.68
24:1Y:48:PHE:O	24:1Y:52:VAL:HG23	1.93	0.68
69:1Y:205:3PE:H292	70:1Y:206:PC1:H3E1	1.75	0.68
69:3C:517:3PE:H322	69:3X:107:3PE:H282	1.74	0.68
49:3E:273:VAL:HG23	49:3E:274:GLY:N	2.08	0.68
51:3G:21:SER:O	51:3G:25:GLN:HG2	1.92	0.68
69:3P:514:3PE:H122	54:3Y:2:LEU:CD1	2.19	0.68
91:4A:609:PGV:H202	66:4L:28:TYR:CG	2.28	0.68
56:4B:132:GLU:HB3	56:4B:137:GLU:HG3	1.74	0.68
12:1L:463:PHE:HB2	69:1L:703:3PE:C27	2.19	0.68
12:1L:591:PHE:HE1	14:1N:110:PRO:O	1.76	0.68
23:1X:34:GLN:HE22	23:1X:116:TRP:NE1	1.92	0.68
69:3R:305:3PE:H3B1	69:3R:305:3PE:H3F1	1.73	0.68
10:1J:95:SER:HB2	69:1J:201:3PE:H3E2	1.75	0.68
13:1M:127:VAL:HG11	69:1N:401:3PE:H3G1	1.74	0.68
13:1M:127:VAL:HG12	69:1N:401:3PE:H3F2	1.76	0.68
35:1j:38:TRP:CE2	69:1k:101:3PE:H382	2.14	0.68
38:1m:91:LEU:HD11	69:1m:202:3PE:H281	1.76	0.68
58:4D:121:LYS:HE2	65:4K:50:PRO:HB2	1.76	0.68
1:1A:23:TRP:CD1	70:1A:202:PC1:O12	2.46	0.68
69:1L:711:3PE:H122	69:1L:712:3PE:H122	1.74	0.68
27:1b:27:LEU:HD13	69:1b:101:3PE:H2G1	1.76	0.68
47:3C:250:LEU:HD22	69:3C:503:3PE:H262	1.75	0.68
47:3C:331:ASP:HA	47:3C:334:THR:HG22	1.74	0.68
69:3C:513:3PE:H232	69:3C:517:3PE:H232	1.76	0.68
1:1A:106:TRP:CE3	69:1A:201:3PE:H251	2.29	0.68
12:1L:602:PHE:HZ	69:1L:706:3PE:H332	1.57	0.68
14:1N:277:ILE:CG1	82:1Y:203:PGT:H161	2.23	0.68
38:1m:92:PHE:CE1	69:1m:203:3PE:C36	2.77	0.68
75:3A:501:CDL:H742	70:3J:106:PC1:H232	1.75	0.68
45:3N:445:ARG:HG2	69:3N:501:3PE:C23	2.20	0.68
69:3Q:503:3PE:H2F2	69:3W:101:3PE:H3C2	1.76	0.68
55:4A:336:PRO:HB2	55:4A:394:VAL:HG11	1.76	0.68
55:4A:406:ASN:HD22	55:4A:409:TRP:HD1	1.42	0.68
91:4A:609:PGV:C25	66:4L:28:TYR:CB	2.71	0.68
91:4C:304:PGV:H281	91:4C:304:PGV:H101	1.75	0.68
61:4G:37:LEU:HD23	69:4G:104:3PE:HN3	1.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:210:GLY:HA2	6:1F:43:TYR:HE2	1.58	0.68
8:1H:169:GLN:O	70:1H:404:PC1:H141	1.93	0.68
14:1N:238:PRO:HB2	69:1N:401:3PE:H11	1.75	0.68
34:1i:18:ARG:HA	39:1n:170:VAL:HG23	1.74	0.68
69:3D:503:3PE:H351	69:3D:503:3PE:H251	1.75	0.68
53:3J:59:LYS:C	53:3J:60:TYR:CA	2.66	0.68
24:1Y:105:ARG:NH1	70:1Y:207:PC1:C11	2.47	0.68
69:1m:202:3PE:O21	69:1m:202:3PE:H332	1.93	0.68
69:3C:513:3PE:C33	69:3X:107:3PE:H262	2.23	0.68
53:3J:17:ARG:CD	69:3J:103:3PE:C1	2.69	0.68
53:3J:46:HIS:HD2	69:3J:101:3PE:H322	1.54	0.68
46:3O:95:LYS:HB2	46:3O:110:GLU:HG3	1.74	0.68
69:3P:517:3PE:H3A1	69:3P:518:3PE:H392	1.75	0.68
49:3R:183:GLU:HB3	49:3R:245:ALA:CB	2.22	0.68
54:3X:15:ARG:NH1	87:3X:102:PEK:P	2.67	0.68
1:1A:23:TRP:HA	70:1A:202:PC1:H121	1.74	0.68
4:1D:349:PHE:CE2	9:1I:82:LEU:HD11	2.28	0.68
14:1N:129:LEU:HD13	75:1N:402:CDL:C54	2.23	0.68
47:3C:231:GLY:HA2	75:3D:504:CDL:H732	1.76	0.68
69:3P:508:3PE:H332	75:3P:513:CDL:C13	2.22	0.68
69:3T:103:3PE:H11	69:3T:103:3PE:HN3	1.57	0.68
20:1U:25:ILE:HG12	20:1U:40:LEU:HD13	1.75	0.68
24:1Y:79:VAL:HG11	69:1Y:214:3PE:H232	1.76	0.68
24:1Y:80:ARG:HE	24:1Y:88:ASN:HD21	1.40	0.68
70:3P:509:PC1:H342	69:3P:514:3PE:H3A2	1.76	0.68
91:4A:606:PGV:H332	67:4M:23:PHE:CD2	2.29	0.68
91:4C:304:PGV:H72	91:4C:304:PGV:H251	1.76	0.68
1:1A:48:ARG:HE	10:1J:78:MET:HA	1.58	0.68
7:1G:46:LEU:O	17:1Q:116:LYS:NZ	2.27	0.68
69:1J:201:3PE:H2B1	69:1Y:210:3PE:H341	1.76	0.68
12:1L:524:ASN:HD22	39:1n:76:PRO:HB2	1.58	0.68
15:1O:187:GLY:O	15:1O:188:ASN:C	2.36	0.68
75:1g:201:CDL:H652	33:1h:35:PRO:HG2	1.75	0.68
34:1i:100:LYS:O	40:1o:49:GLN:NE2	2.27	0.68
53:3J:56:ILE:O	53:3J:58:HIS:C	2.37	0.68
75:3P:513:CDL:H511	51:3T:40:ARG:NH2	2.09	0.68
69:3P:515:3PE:H3G1	70:3T:102:PC1:H2I3	1.75	0.68
49:3R:197:ASP:HB3	49:3R:248:ARG:NH1	2.09	0.68
5:1E:103:CYS:SG	72:1E:301:FES:FE1	1.85	0.67
7:1G:490:MET:HE2	7:1G:490:MET:HA	1.76	0.67
12:1L:504:LEU:CD2	64:4J:30:ILE:HD11	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:92:PHE:CE1	69:1m:203:3PE:H252	2.29	0.67
45:3A:124:ASP:OD1	45:3A:179:ARG:HD2	1.93	0.67
49:3R:242:HIS:HB2	49:3R:250:ARG:HG2	1.76	0.67
2:1B:177:TYR:HA	70:1B:202:PC1:H261	1.70	0.67
69:1N:401:3PE:N	69:1N:401:3PE:H12	2.10	0.67
15:1O:30:ASN:HD22	15:1O:179:ILE:HD13	1.59	0.67
69:1Y:209:3PE:H121	51:3T:35:PRO:HB3	1.74	0.67
69:1d:201:3PE:C2G	69:1d:201:3PE:C3E	2.71	0.67
32:1g:59:ARG:NH2	69:1g:203:3PE:C1	2.57	0.67
48:3D:129:HIS:HE1	48:3D:199:PRO:HD2	1.58	0.67
52:3H:77:GLU:C	52:3H:78:ASP:N	2.52	0.67
69:3P:504:3PE:H352	69:3Y:103:3PE:H331	1.77	0.67
69:3P:510:3PE:H2I3	51:3T:54:VAL:CG2	2.24	0.67
53:3W:23:LEU:HD23	69:3W:103:3PE:H3A2	1.74	0.67
2:1B:71:ARG:NH2	9:1I:49:ASN:OD1	2.27	0.67
69:1B:204:3PE:H391	69:1B:205:3PE:H3B1	1.74	0.67
10:1J:23:LYS:HB3	11:1K:28:SER:OG	1.95	0.67
12:1L:562:LEU:HD22	69:1L:705:3PE:H3B1	1.75	0.67
12:1L:603:ASN:HB2	69:1L:706:3PE:O13	1.94	0.67
69:1f:103:3PE:H3B1	69:1g:202:3PE:H2I3	1.75	0.67
69:3C:504:3PE:H262	48:3D:105:LEU:HD13	1.76	0.67
69:3C:508:3PE:H3A1	69:3C:508:3PE:H2E1	1.76	0.67
53:3J:59:LYS:CA	53:3J:60:TYR:N	2.57	0.67
69:3P:508:3PE:H3F1	69:3P:508:3PE:H3B2	1.76	0.67
59:4E:76:GLY:O	59:4E:79:LYS:NZ	2.27	0.67
70:1B:203:PC1:H2	69:1B:204:3PE:H32	1.75	0.67
14:1N:329:MET:HE1	75:1N:402:CDL:H781	1.75	0.67
46:3B:306:PRO:HA	49:3I:52:ARG:HB2	1.76	0.67
47:3C:299:LEU:CD1	69:3C:512:3PE:C3I	2.72	0.67
45:3N:86:LEU:HD13	45:3N:99:ILE:HG12	1.75	0.67
69:3P:503:3PE:H382	69:3P:505:3PE:C35	2.25	0.67
49:3R:224:PRO:HB3	49:3R:243:TYR:CE2	2.29	0.67
51:3T:64:GLN:HB3	51:3T:68:LYS:NZ	2.08	0.67
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.76	0.67
2:1B:176:TRP:CZ3	70:1B:202:PC1:C26	2.78	0.67
7:1G:470:VAL:HG12	7:1G:490:MET:HE1	1.77	0.67
46:3B:35:ILE:HD11	46:3B:220:ALA:CB	2.25	0.67
69:3C:513:3PE:H3A2	69:3C:513:3PE:H2E2	1.76	0.67
48:3D:245:GLN:HG2	52:3H:84:PHE:HZ	1.58	0.67
46:3O:51:ILE:HG12	46:3O:204:MET:HG2	1.74	0.67
54:3X:44:TRP:CE2	69:3X:108:3PE:H221	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:3Y:4:ARG:NH1	75:3Y:106:CDL:OA3	2.26	0.67
7:1G:465:ALA:HB2	7:1G:654:GLN:HG3	1.77	0.67
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.76	0.67
14:1N:325:LEU:H	75:1d:205:CDL:PA1	2.18	0.67
69:1Y:215:3PE:H2E1	70:3T:102:PC1:H3A1	1.75	0.67
42:1q:6:VAL:HG12	75:1q:201:CDL:OA9	1.94	0.67
69:3C:514:3PE:H381	69:3C:514:3PE:H261	1.75	0.67
49:3E:219:HIS:HB3	72:3E:301:FES:S2	2.33	0.67
46:3O:196:GLN:HA	46:3O:227:ARG:CD	2.22	0.67
49:3R:179:ARG:HB3	49:3R:183:GLU:HB2	1.76	0.67
53:3W:56:ILE:HG12	53:3W:57:LYS:HG3	1.77	0.67
10:1J:87:LYS:HD2	10:1J:90:PHE:HD2	1.59	0.67
12:1L:541:ASN:HB3	69:1L:701:3PE:H272	1.77	0.67
12:1L:602:PHE:CZ	69:1L:706:3PE:O32	2.48	0.67
38:1m:82:THR:HB	38:1m:83:PRO:HD2	1.75	0.67
38:1m:96:PRO:HG3	69:1m:203:3PE:H2A2	1.76	0.67
39:1n:54:LYS:HD2	45:3N:20:ASP:O	1.91	0.67
69:3C:515:3PE:H2E1	69:3C:515:3PE:H392	1.76	0.67
49:3E:155:LYS:CG	49:3E:274:GLY:OXT	2.41	0.67
46:3O:129:ALA:N	46:3O:130:PRO:HD3	2.09	0.67
54:3Y:33:VAL:HG21	69:3Y:105:3PE:C2G	2.23	0.67
54:3Y:41:ILE:HD12	69:3Y:105:3PE:H291	1.77	0.67
55:4A:289:ALA:C	55:4A:291:HIS:N	2.52	0.67
55:4A:407:GLN:NE2	91:4A:606:PGV:H062	2.08	0.67
12:1L:463:PHE:CE2	69:1k:101:3PE:H3I3	2.30	0.67
32:1g:75:THR:HG21	33:1h:36:VAL:HG11	1.77	0.67
41:1p:140:ASP:O	41:1p:161:ARG:NH2	2.27	0.67
49:3E:155:LYS:CE	49:3E:274:GLY:OXT	2.42	0.67
45:3N:444:LEU:HD21	69:3N:503:3PE:H112	1.76	0.67
69:3N:501:3PE:C29	75:3N:502:CDL:H532	2.25	0.67
69:3P:516:3PE:H2E1	70:3T:102:PC1:H2C2	1.77	0.67
87:3X:102:PEK:N	60:4F:1:ALA:HB2	2.09	0.67
24:1Y:87:LEU:N	70:1Y:202:PC1:H341	2.10	0.67
40:1o:77:LEU:HD12	69:1o:201:3PE:H262	1.74	0.67
45:3A:436:ARG:HD3	47:3C:222:PRO:HD3	1.76	0.67
49:3I:77:ARG:HB3	49:3I:77:ARG:HH11	1.60	0.67
46:3O:350:GLY:HA2	46:3O:411:ILE:HD13	1.77	0.67
56:4B:30:ILE:HG21	56:4B:76:ILE:HD11	1.76	0.67
69:1J:203:3PE:H121	69:1Y:210:3PE:O12	1.94	0.67
14:1N:336:VAL:HG21	69:1d:203:3PE:C2H	2.25	0.67
24:1Y:5:LEU:CG	69:1Y:211:3PE:H331	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1Y:215:3PE:H2A2	69:1Y:216:3PE:H2E2	1.77	0.67
75:1q:201:CDL:H162	75:1q:201:CDL:H331	1.77	0.67
47:3C:360:LEU:CA	69:3C:512:3PE:H2I2	2.23	0.67
46:3O:283:PRO:HG3	49:3V:57:GLY:HA3	1.76	0.67
55:4A:208:MET:CE	57:4C:100:ALA:HB2	2.25	0.67
56:4B:7:LEU:HD11	75:4B:302:CDL:C71	2.25	0.67
9:1I:87:CYS:SG	71:1I:201:SF4:FE1	1.87	0.66
35:1j:38:TRP:CZ2	69:1k:101:3PE:C38	2.78	0.66
43:1r:8:GLN:O	43:1r:11:ARG:HG3	1.94	0.66
48:3D:171:ARG:NH1	48:3D:174:LYS:HG3	2.09	0.66
69:3N:503:3PE:H3H1	69:3R:302:3PE:H3H1	1.76	0.66
47:3P:8:HIS:CD2	47:3P:11:MET:HG2	2.30	0.66
47:3P:249:LEU:HD12	69:3P:520:3PE:C2	2.24	0.66
57:4C:149:HIS:HA	57:4C:152:MET:HE2	1.76	0.66
2:1B:104:TYR:O	2:1B:111:ARG:NH1	2.28	0.66
7:1G:150:MET:HE2	7:1G:150:MET:HA	1.77	0.66
31:1f:14:ILE:HD11	69:1f:101:3PE:H2B2	1.75	0.66
38:1m:99:PHE:CD2	69:1m:205:3PE:C3G	2.74	0.66
51:3G:33:THR:O	69:3G:103:3PE:H122	1.96	0.66
56:4B:35:SER:HB2	75:4B:302:CDL:H402	1.78	0.66
57:4C:242:TRP:O	57:4C:245:VAL:HG22	1.95	0.66
29:1d:8:ARG:CG	70:1d:204:PC1:C24	2.74	0.66
75:1g:201:CDL:H772	33:1h:34:ILE:CG2	2.25	0.66
75:3N:502:CDL:H181	69:3P:511:3PE:H2I3	1.77	0.66
69:3W:103:3PE:H382	54:3X:23:MET:HE1	1.76	0.66
54:3Y:23:MET:HE2	69:3Y:101:3PE:C34	2.25	0.66
55:4A:418:PHE:CE2	91:4A:608:PGV:H141	2.30	0.66
57:4C:22:LEU:HD22	64:4J:43:THR:HG21	1.78	0.66
7:1G:11:VAL:HG11	7:1G:73:VAL:HB	1.76	0.66
12:1L:464:ALA:CB	69:1L:703:3PE:H2A2	2.24	0.66
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	1.76	0.66
13:1M:430:PHE:HB2	13:1M:433:GLU:HG3	1.78	0.66
69:3A:503:3PE:H122	69:3C:516:3PE:HN1	1.57	0.66
47:3C:359:PHE:CD2	69:3C:511:3PE:H3C1	2.30	0.66
47:3C:363:LEU:HB2	69:3C:512:3PE:H2I1	1.77	0.66
69:3E:302:3PE:H2G2	70:3J:106:PC1:H291	1.78	0.66
75:3F:201:CDL:H792	69:3G:109:3PE:H341	1.78	0.66
51:3G:69:GLU:HA	51:3G:72:LYS:HE3	1.75	0.66
53:3J:53:TRP:CH2	53:3J:60:TYR:CD2	2.84	0.66
69:3P:510:3PE:H2F2	51:3T:54:VAL:CG2	2.25	0.66
69:3P:519:3PE:H2A1	69:3P:520:3PE:H362	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:3X:103:CDL:H241	75:3X:103:CDL:H873	1.77	0.66
5:1E:55:GLN:HE22	5:1E:90:TYR:HA	1.59	0.66
16:1P:270:PHE:HE2	16:1P:278:TRP:HE3	1.44	0.66
24:1Y:90:PHE:HB2	70:1Y:202:PC1:H352	1.77	0.66
24:1Y:109:ILE:HG23	70:1Y:206:PC1:H351	1.76	0.66
45:3A:30:SER:HB2	45:3A:32:GLN:HG3	1.78	0.66
49:3E:187:GLU:O	49:3E:190:VAL:HB	1.94	0.66
47:3P:306:MET:HG2	69:3P:514:3PE:H222	1.77	0.66
54:3Y:6:LEU:HD23	69:3Y:107:3PE:C2D	2.26	0.66
91:4A:608:PGV:H332	75:4B:302:CDL:H451	1.77	0.66
2:1B:177:TYR:HB2	70:1B:202:PC1:H261	1.75	0.66
6:1F:343:ILE:HD11	6:1F:425:GLU:HG2	1.78	0.66
24:1Y:113:ALA:CB	70:1Y:206:PC1:H372	2.26	0.66
69:1Y:215:3PE:H331	69:1Y:216:3PE:C37	2.25	0.66
40:1o:76:PHE:HE1	69:1o:201:3PE:H2B1	1.60	0.66
47:3C:253:PRO:O	48:3D:207:ALA:HA	1.96	0.66
49:3R:170:ARG:HG2	49:3R:274:GLY:O	1.95	0.66
75:4C:306:CDL:H722	75:4C:306:CDL:HB61	1.77	0.66
31:1f:17:PRO:CB	69:1f:102:3PE:H2G2	2.26	0.66
46:3B:73:SER:O	46:3B:74:SER:HB3	1.96	0.66
75:3P:513:CDL:H572	75:3T:101:CDL:H111	1.77	0.66
52:3U:34:ARG:O	52:3U:38:GLU:HG3	1.96	0.66
15:1O:60:ASP:OD1	15:1O:60:ASP:N	2.29	0.66
24:1Y:39:SER:CA	69:1Y:204:3PE:H11	2.24	0.66
24:1Y:87:LEU:HD13	69:1Y:212:3PE:C33	2.16	0.66
69:1f:102:3PE:H2	69:1g:202:3PE:H321	1.77	0.66
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.27	0.66
47:3C:4:ILE:CD1	69:3C:515:3PE:O32	2.44	0.66
48:3D:227:THR:CG2	52:3H:69:VAL:HB	2.26	0.66
49:3E:235:TYR:CE2	49:3E:237:PRO:HB3	2.30	0.66
47:3P:320:LEU:HD23	70:3T:102:PC1:H222	1.78	0.66
91:4C:302:PGV:H011	91:4C:302:PGV:H042	1.76	0.66
4:1D:50:ASN:HB2	4:1D:65:VAL:HG22	1.78	0.66
15:1O:135:LEU:HD22	15:1O:152:TYR:CD2	2.31	0.66
16:1P:99:TRP:CH2	16:1P:276:GLU:HG3	2.31	0.66
69:1g:203:3PE:H351	69:1g:203:3PE:H232	1.78	0.66
69:3G:108:3PE:H342	69:3G:108:3PE:C25	2.24	0.66
47:3P:297:SER:O	69:3P:519:3PE:H3I1	1.95	0.66
49:3R:176:VAL:HG22	49:3R:212:ILE:HG13	1.78	0.66
49:3R:211:VAL:HG11	49:3R:245:ALA:O	1.96	0.66
49:3R:231:PHE:CG	49:3R:250:ARG:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3T:103:3PE:H322	69:3T:103:3PE:H2I1	1.76	0.66
9:1I:84:GLU:HG3	9:1I:92:ILE:O	1.96	0.65
12:1L:159:HIS:HB2	13:1M:416:ARG:HB3	1.78	0.65
12:1L:545:SER:OG	13:1M:274:SER:O	2.14	0.65
14:1N:317:PHE:HZ	15:1O:106:LEU:HD11	1.61	0.65
70:1h:202:PC1:H391	69:1h:204:3PE:H362	1.78	0.65
47:3C:292:LEU:CD1	69:3C:513:3PE:H282	2.26	0.65
55:4A:193:VAL:HG21	91:4A:607:PGV:H251	1.76	0.65
69:1L:702:3PE:O32	69:1L:702:3PE:H222	1.96	0.65
24:1Y:62:SER:OG	69:1Y:208:3PE:C32	2.44	0.65
69:1Y:205:3PE:H321	70:1Y:206:PC1:H3A1	1.78	0.65
70:1Y:206:PC1:H121	38:1m:81:PRO:HD3	1.78	0.65
75:1Y:217:CDL:H161	70:3T:102:PC1:H31	1.76	0.65
45:3A:19:LEU:HB2	45:3A:21:ASN:OD1	1.96	0.65
45:3A:358:LYS:O	45:3A:362:ARG:HG3	1.95	0.65
69:3X:105:3PE:H222	69:3X:105:3PE:C11	2.26	0.65
64:4J:41:GLY:C	91:4J:101:PGV:H292	2.22	0.65
5:1E:148:CYS:SG	72:1E:301:FES:FE2	1.85	0.65
69:1L:712:3PE:H231	69:1l:204:3PE:H231	1.76	0.65
50:3F:94:LYS:HB3	50:3F:96:GLU:OE1	1.95	0.65
75:3F:201:CDL:H602	75:3F:201:CDL:H811	1.78	0.65
51:3G:44:ARG:NH2	69:3G:105:3PE:HN1	1.80	0.65
69:3R:305:3PE:H32	51:3T:26:PHE:HD1	1.61	0.65
14:1N:109:SER:HB3	14:1N:157:MET:HG2	1.78	0.65
15:1O:83:TYR:HB2	15:1O:190:HIS:HB3	1.79	0.65
32:1g:100:ARG:NH1	32:1g:107:LEU:O	2.29	0.65
69:3N:501:3PE:H3B1	47:3P:14:ILE:HD13	1.78	0.65
1:1A:37:TYR:OH	4:1D:54:GLN:OE1	2.14	0.65
7:1G:126:ASP:OD1	43:1r:56:ARG:NH1	2.29	0.65
11:1K:27:MET:HE2	11:1K:78:LEU:HD13	1.78	0.65
12:1L:471:ASN:CG	69:1o:201:3PE:H2H1	2.22	0.65
69:1L:709:3PE:O32	33:1h:26:ARG:HG2	1.96	0.65
75:1Y:217:CDL:H271	69:3S:201:3PE:H3D2	1.78	0.65
29:1d:8:ARG:CD	70:1d:204:PC1:C23	2.68	0.65
69:1k:101:3PE:H291	69:1k:101:3PE:H3B1	1.79	0.65
45:3N:277:ILE:HB	45:3N:309:THR:HG21	1.78	0.65
46:3O:278:VAL:HG11	46:3O:352:LEU:HD13	1.79	0.65
52:3U:20:VAL:HA	52:3U:23:GLN:NE2	2.11	0.65
53:3W:10:LEU:HD12	53:3W:14:LEU:HD12	1.77	0.65
57:4C:231:HIS:CG	91:4C:305:PGV:O06	2.49	0.65
6:1F:203:PRO:O	6:1F:404:ILE:HD11	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:301:ILE:HD11	12:1L:422:TYR:HB2	1.79	0.65
25:1Z:10:MET:HE3	25:1Z:11:PRO:HD2	1.77	0.65
85:3C:501:HEM:HBC2	85:3C:501:HEM:HMC1	1.77	0.65
69:3J:104:3PE:H3G2	69:3J:105:3PE:H392	1.77	0.65
69:3X:108:3PE:H392	69:4G:104:3PE:H392	1.78	0.65
8:1H:306:SER:HB3	27:1b:32:PRO:HG3	1.79	0.65
13:1M:29:VAL:HG11	69:1g:202:3PE:H2D2	1.78	0.65
24:1Y:80:ARG:NH1	69:1Y:212:3PE:C21	2.57	0.65
24:1Y:99:THR:HG22	70:1Y:207:PC1:H342	1.78	0.65
45:3A:21:ASN:HB2	45:3A:220:SER:O	1.97	0.65
69:3J:104:3PE:H231	69:3J:104:3PE:H2	1.77	0.65
60:4F:18:ARG:O	60:4F:22:MET:HG2	1.97	0.65
2:1B:42:ARG:NH2	70:1B:203:PC1:O12	2.30	0.65
4:1D:130:PRO:HG2	4:1D:135:GLN:HE21	1.60	0.65
7:1G:243:ARG:HG2	7:1G:244:THR:HG23	1.78	0.65
7:1G:627:SER:OG	7:1G:629:ASN:ND2	2.30	0.65
10:1J:17:PHE:CD2	11:1K:14:ILE:HD11	2.31	0.65
12:1L:357:ARG:HG2	39:1n:31:VAL:HG22	1.78	0.65
69:1m:202:3PE:C35	51:3T:34:ILE:HD12	2.26	0.65
48:3Q:15:ARG:HD3	69:3Q:504:3PE:O12	1.97	0.65
54:3X:23:MET:O	54:3X:27:VAL:HG23	1.97	0.65
54:3X:44:TRP:CE3	69:3X:108:3PE:C38	2.80	0.65
69:4G:101:3PE:C32	69:4G:104:3PE:H232	2.26	0.65
7:1G:366:THR:HG23	7:1G:370:GLY:HA3	1.79	0.65
7:1G:451:VAL:HG22	7:1G:489:VAL:HG12	1.77	0.65
9:1I:78:ILE:HA	9:1I:104:ARG:O	1.97	0.65
10:1J:18:VAL:HG13	69:1J:203:3PE:H391	1.77	0.65
24:1Y:75:ILE:HG21	69:1Y:201:3PE:C27	2.25	0.65
69:1g:202:3PE:H31	69:1g:202:3PE:HN2	1.62	0.65
46:3B:227:ARG:HG3	46:3B:229:GLY:H	1.61	0.65
69:3C:508:3PE:H3C2	69:3G:109:3PE:H331	1.79	0.65
48:3D:160:ASP:HB2	48:3D:171:ARG:HG2	1.77	0.65
49:3E:191:GLU:HG3	49:3E:194:GLN:H	1.61	0.65
46:3O:44:ALA:HA	46:3O:112:LEU:HA	1.79	0.65
69:3W:102:3PE:H361	69:3X:101:3PE:H372	1.79	0.65
10:1J:87:LYS:HG2	69:1J:201:3PE:N	2.12	0.65
69:1L:703:3PE:C1	40:1o:77:LEU:HD11	2.26	0.65
13:1M:10:MET:CE	69:1f:104:3PE:C38	2.75	0.65
69:1d:206:3PE:H372	69:1f:104:3PE:C29	2.26	0.65
47:3C:238:ILE:HD12	69:3C:505:3PE:H2F2	1.77	0.65
69:3G:103:3PE:H112	69:3G:104:3PE:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:307:PHE:CD2	49:3V:52:ARG:HD2	2.31	0.65
4:1D:348:HIS:HE1	9:1I:125:ALA:O	1.80	0.64
10:1J:17:PHE:HB3	11:1K:14:ILE:CD1	2.27	0.64
12:1L:13:ILE:HG13	34:1i:81:ILE:HD11	1.79	0.64
12:1L:142:ILE:CG2	75:1L:704:CDL:H791	2.27	0.64
13:1M:197:LEU:O	13:1M:201:MET:HG2	1.97	0.64
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.79	0.64
29:1d:60:ARG:HG2	75:1d:205:CDL:HB32	1.77	0.64
75:1d:202:CDL:H361	75:1d:202:CDL:H531	1.79	0.64
30:1e:18:THR:HG22	30:1e:19:ILE:HG23	1.79	0.64
69:3P:507:3PE:H222	54:3Y:38:TRP:CG	2.33	0.64
69:3P:519:3PE:H351	69:3P:519:3PE:H272	1.79	0.64
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.78	0.64
75:1d:205:CDL:H321	75:1d:205:CDL:HA4	1.79	0.64
69:1m:203:3PE:H3C2	69:1m:205:3PE:H3I1	1.79	0.64
50:3F:63:PRO:HD3	50:3F:105:TYR:OH	1.96	0.64
69:3X:107:3PE:O32	69:4G:104:3PE:H231	1.97	0.64
69:3Y:102:3PE:H3D1	69:3Y:105:3PE:H3G1	1.77	0.64
5:1E:169:ILE:HA	5:1E:172:ILE:HD12	1.79	0.64
8:1H:99:ASN:CG	70:1H:403:PC1:H152	2.20	0.64
11:1K:15:ALA:HB1	11:1K:36:MET:HG3	1.79	0.64
48:3D:293:MET:HE3	69:3E:303:3PE:O22	1.97	0.64
45:3N:114:ALA:O	45:3N:118:GLN:HB2	1.97	0.64
55:4A:138:HIS:O	55:4A:213:ARG:NH2	2.30	0.64
68:4N:2:LEU:N	68:4N:2:LEU:HD12	2.11	0.64
4:1D:226:GLU:OE1	25:1Z:23:ARG:NH1	2.30	0.64
10:1J:3:MET:HE1	25:1Z:133:ILE:HD11	1.79	0.64
12:1L:595:ILE:HG12	14:1N:100:MET:HE3	1.80	0.64
14:1N:54:GLU:OE1	14:1N:58:LYS:NZ	2.29	0.64
15:1O:77:CYS:HB2	15:1O:96:LEU:CB	2.28	0.64
75:1g:201:CDL:OB9	33:1h:30:LEU:CB	2.45	0.64
38:1m:99:PHE:CD2	69:1m:205:3PE:H3I2	2.33	0.64
47:3C:299:LEU:HD12	69:3C:512:3PE:H3I3	1.79	0.64
53:3J:36:PHE:HA	69:3J:104:3PE:H3D1	1.78	0.64
54:3Y:6:LEU:CD2	69:3Y:107:3PE:C2D	2.75	0.64
55:4A:321:PHE:HA	55:4A:324:LEU:HD12	1.79	0.64
70:1H:404:PC1:O14	70:1H:404:PC1:H121	1.95	0.64
13:1M:97:THR:O	13:1M:101:LEU:HG	1.98	0.64
69:3N:503:3PE:H292	69:3R:304:3PE:H2I3	1.78	0.64
49:3R:163:LYS:O	49:3R:177:ARG:HA	1.98	0.64
69:3X:101:3PE:H352	69:3X:101:3PE:H12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:22:PHE:CD1	91:4A:609:PGV:H12	2.26	0.64
56:4B:104:TRP:NE1	56:4B:200:CYS:O	2.28	0.64
2:1B:42:ARG:HH12	70:1B:203:PC1:P	2.19	0.64
28:1c:26:PHE:HE2	75:1d:205:CDL:H802	1.63	0.64
70:1h:202:PC1:H111	70:1h:202:PC1:H2	1.80	0.64
49:3E:213:LEU:HD13	49:3E:247:GLY:HA3	1.78	0.64
49:3E:263:TYR:HB2	49:3E:272:ILE:H	1.60	0.64
69:3G:101:3PE:O22	69:3G:108:3PE:H32	1.96	0.64
55:4A:22:PHE:HD1	91:4A:609:PGV:C12	2.10	0.64
91:4A:609:PGV:H321	91:4A:609:PGV:H132	1.80	0.64
15:1O:31:ILE:HD12	15:1O:31:ILE:H	1.63	0.64
46:3B:325:TYR:CD1	49:3I:59:ALA:HA	2.33	0.64
49:3E:244:ASP:HB2	49:3E:250:ARG:CG	2.28	0.64
75:3F:201:CDL:H391	75:3F:201:CDL:H352	1.79	0.64
53:3J:54:LYS:CA	53:3J:57:LYS:HE2	2.27	0.64
50:3S:12:TRP:HA	50:3S:12:TRP:CE3	2.33	0.64
54:3Y:4:ARG:NH2	69:3Y:107:3PE:P	2.71	0.64
57:4C:62:ILE:CG1	91:4C:305:PGV:H21	2.28	0.64
1:1A:23:TRP:O	70:1A:202:PC1:H121	1.98	0.64
70:1B:202:PC1:C22	16:1P:275:PHE:CE1	2.74	0.64
75:3N:502:CDL:H602	69:3N:503:3PE:H2F1	1.78	0.64
49:3R:161:GLU:HA	49:3R:178:HIS:HB3	1.79	0.64
54:3Y:5:PHE:CD1	75:3Y:106:CDL:H312	2.32	0.64
12:1L:519:THR:HG21	69:1L:707:3PE:H232	1.79	0.64
16:1P:270:PHE:HD2	16:1P:278:TRP:HB2	1.61	0.64
27:1b:27:LEU:CD1	69:1b:101:3PE:C2G	2.76	0.64
28:1c:34:GLN:HE22	69:1d:203:3PE:C12	2.01	0.64
31:1f:22:PHE:HB2	69:1f:104:3PE:C3B	2.14	0.64
32:1g:43:ASP:OD1	39:1n:107:HIS:NE2	2.31	0.64
38:1m:126:ILE:HG22	41:1p:139:GLN:HG3	1.79	0.64
49:3E:213:LEU:CD1	49:3E:247:GLY:HA3	2.28	0.64
75:3X:103:CDL:H591	69:3X:105:3PE:H341	1.80	0.64
69:1A:201:3PE:H321	69:1b:101:3PE:H11	1.79	0.64
15:1O:294:GLN:O	15:1O:298:GLU:HG3	1.97	0.64
19:1S:68:TYR:HB2	19:1S:72:GLN:HB2	1.79	0.64
24:1Y:5:LEU:CD2	69:1Y:211:3PE:C32	2.65	0.64
24:1Y:113:ALA:HB2	70:1Y:206:PC1:H372	1.80	0.64
34:1i:83:TYR:CD2	75:1i:201:CDL:H531	2.32	0.64
45:3A:242:ARG:HB2	51:3G:17:THR:HG22	1.80	0.64
47:3C:284:ILE:HG23	69:3C:512:3PE:H232	1.80	0.64
47:3C:287:LYS:CB	69:3C:513:3PE:H122	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:159:ILE:HG21	49:3E:176:VAL:O	1.97	0.64
49:3R:181:LYS:O	49:3R:182:LYS:C	2.40	0.64
49:3R:196:ARG:HH11	49:3R:196:ARG:C	2.05	0.64
69:1B:205:3PE:H341	75:1q:202:CDL:H542	1.81	0.63
69:1L:711:3PE:H251	69:1L:712:3PE:H31	1.79	0.63
69:1L:712:3PE:H32	69:1l:204:3PE:H332	1.79	0.63
32:1g:59:ARG:HH22	69:1g:203:3PE:C1	2.12	0.63
49:3E:161:GLU:HA	49:3E:178:HIS:HB3	1.79	0.63
45:3N:223:TYR:O	45:3N:224:VAL:C	2.40	0.63
45:3N:444:LEU:HD22	69:3N:503:3PE:H112	1.78	0.63
46:3O:157:ALA:O	46:3O:161:GLU:HG2	1.98	0.63
69:3P:506:3PE:O12	69:3P:506:3PE:H122	1.96	0.63
69:3P:514:3PE:N	54:3Y:2:LEU:HD13	2.12	0.63
57:4C:54:MET:HG2	91:4C:301:PGV:H61	1.79	0.63
4:1D:68:LEU:HD21	4:1D:411:LEU:HD13	1.80	0.63
13:1M:220:HIS:CE1	13:1M:231:LEU:HB3	2.33	0.63
29:1d:33:TYR:HD1	75:1d:202:CDL:H411	1.61	0.63
47:3C:281:LEU:HB2	47:3C:294:LEU:HB2	1.80	0.63
47:3C:306:MET:HA	69:3C:506:3PE:H122	1.79	0.63
49:3E:201:ASP:O	49:3E:205:VAL:HG23	1.97	0.63
49:3E:219:HIS:ND1	49:3E:222:CYS:HB2	2.14	0.63
49:3R:201:ASP:O	49:3R:205:VAL:HG12	1.97	0.63
5:1E:93:LYS:HG3	5:1E:94:PRO:HD2	1.78	0.63
8:1H:107:ALA:O	8:1H:111:LEU:HG	1.98	0.63
14:1N:325:LEU:HD11	69:1e:201:3PE:H252	1.80	0.63
16:1P:194:ILE:HD13	16:1P:260:HIS:HA	1.81	0.63
33:1h:36:VAL:HG23	70:1h:202:PC1:C2I	2.29	0.63
34:1i:84:TYR:CD2	75:1i:201:CDL:H351	2.33	0.63
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.31	0.63
69:3C:509:3PE:H342	69:3X:107:3PE:H371	1.81	0.63
53:3J:17:ARG:HB2	53:3J:20:THR:HG22	1.80	0.63
48:3Q:218:LEU:CD2	69:3R:305:3PE:H372	2.26	0.63
49:3R:206:LYS:HB2	49:3R:265:PHE:HD2	1.64	0.63
91:4A:607:PGV:H031	75:4C:306:CDL:H473	1.80	0.63
62:4H:43:MET:HA	62:4H:46:LYS:HG2	1.81	0.63
69:1N:401:3PE:H3E2	69:1N:401:3PE:H2C1	1.80	0.63
15:1O:56:ILE:HD11	15:1O:96:LEU:HD12	1.80	0.63
24:1Y:98:LEU:CD2	70:1Y:207:PC1:H241	2.28	0.63
47:3C:26:ASN:HD21	47:3C:207:ASN:HD22	1.46	0.63
47:3C:289:GLY:CA	69:3C:512:3PE:H351	2.27	0.63
47:3C:368:ILE:CG2	69:3C:507:3PE:H271	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3C:506:3PE:H2E1	69:3C:507:3PE:H371	1.81	0.63
69:3C:509:3PE:O21	69:3X:107:3PE:H322	1.98	0.63
48:3D:232:ARG:NH1	49:3R:237:PRO:HB2	2.13	0.63
75:3N:502:CDL:C54	69:3P:511:3PE:H362	2.27	0.63
47:3P:303:LEU:HD21	69:3P:514:3PE:H2E1	1.79	0.63
69:3Y:104:3PE:H3H2	75:3Y:106:CDL:H812	1.80	0.63
10:1J:17:PHE:HD2	11:1K:14:ILE:HD11	1.63	0.63
12:1L:468:ILE:HD11	69:1L:703:3PE:H2H1	1.81	0.63
69:1Y:201:3PE:H3A2	51:3T:56:TYR:HB2	1.81	0.63
75:1Y:217:CDL:H211	75:1Y:217:CDL:H361	1.80	0.63
75:1Y:217:CDL:H221	70:3T:102:PC1:H341	1.80	0.63
69:1d:201:3PE:C2G	69:1d:201:3PE:C3F	2.76	0.63
75:1g:201:CDL:H271	69:1g:202:3PE:H2I2	1.81	0.63
69:3C:506:3PE:H342	69:3C:506:3PE:H292	1.80	0.63
69:3C:513:3PE:H32	69:3C:513:3PE:H342	1.81	0.63
45:3N:297:VAL:HG13	47:3P:1:MET:HG3	1.80	0.63
45:3N:381:ARG:NH1	45:3N:381:ARG:HB3	2.13	0.63
45:3N:399:ILE:O	45:3N:402:VAL:HG12	1.98	0.63
69:3P:504:3PE:H322	69:3Y:103:3PE:H331	1.81	0.63
69:1A:201:3PE:H392	69:1b:101:3PE:H262	1.80	0.63
7:1G:306:MET:HE2	7:1G:542:PHE:HB2	1.79	0.63
10:1J:151:THR:HG21	70:1J:202:PC1:H321	1.80	0.63
12:1L:213:LEU:HB2	12:1L:273:VAL:HG21	1.81	0.63
12:1L:517:SER:OG	69:1L:708:3PE:C1	2.32	0.63
13:1M:425:ASN:HB2	38:1m:57:GLY:HA2	1.80	0.63
27:1b:27:LEU:CD1	69:1b:101:3PE:C2D	2.53	0.63
69:1d:201:3PE:C2F	69:1d:201:3PE:C3E	2.76	0.63
31:1f:21:VAL:CG2	69:1f:104:3PE:H3E1	2.18	0.63
45:3A:414:TYR:O	45:3A:418:GLN:HG3	1.99	0.63
69:3A:502:3PE:H241	69:3A:502:3PE:H2A2	1.81	0.63
49:3E:179:ARG:CD	49:3E:211:VAL:HB	2.29	0.63
49:3E:237:PRO:O	48:3Q:144:ARG:HG2	1.98	0.63
48:3Q:210:MET:HE1	53:3W:40:ALA:CB	2.29	0.63
69:3W:101:3PE:H3E1	69:3W:102:3PE:H261	1.80	0.63
1:1A:35:SER:O	2:1B:81:ARG:NH2	2.32	0.63
13:1M:282:LEU:HD13	13:1M:342:MET:HG3	1.81	0.63
14:1N:2:ASN:HB3	14:1N:5:ILE:HD12	1.81	0.63
24:1Y:31:THR:HG21	69:1Y:208:3PE:H2C1	1.80	0.63
24:1Y:98:LEU:HD11	69:1Y:212:3PE:H2F2	1.81	0.63
38:1m:24:ILE:O	45:3N:227:ALA:CA	2.45	0.63
49:3E:195:LEU:HD22	49:3E:250:ARG:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:152:TYR:CE1	49:3R:83:ILE:HG12	2.33	0.63
48:3Q:37:CYS:HG	86:3Q:501:HEC:HBB3	1.60	0.63
48:3Q:230:LEU:O	48:3Q:233:ARG:HG2	1.99	0.63
56:4B:65:TRP:HB3	93:4B:303:PSC:H1	1.81	0.63
59:4E:52:LEU:HD22	59:4E:98:ILE:HD13	1.80	0.63
11:1K:95:LEU:HD23	11:1K:95:LEU:H	1.63	0.63
69:1Y:215:3PE:H3C2	70:3T:102:PC1:H3A2	1.80	0.63
49:3E:141:SER:OG	69:3E:302:3PE:H321	1.99	0.63
45:3N:283:THR:HA	46:3O:143:GLN:NE2	2.13	0.63
48:3Q:75:ASN:OD1	48:3Q:79:GLU:HG2	1.99	0.63
49:3R:248:ARG:HD2	49:3R:257:ASN:HD22	1.64	0.63
69:3R:305:3PE:H231	69:3T:103:3PE:H12	1.79	0.63
55:4A:21:LEU:HD12	91:4A:609:PGV:H62	1.81	0.63
56:4B:69:PRO:HG3	93:4B:303:PSC:H171	1.81	0.63
5:1E:210:GLY:HA2	6:1F:43:TYR:CE2	2.34	0.63
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.81	0.63
12:1L:486:MET:O	12:1L:489:THR:OG1	2.17	0.63
14:1N:272:LYS:HD3	33:1h:108:LEU:HD21	1.81	0.63
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.31	0.63
45:3N:237:THR:HG21	51:3T:18:LEU:HD11	1.80	0.63
54:3Y:4:ARG:NH2	69:3Y:107:3PE:C1	2.62	0.63
14:1N:246:VAL:HG21	69:1N:401:3PE:H282	1.81	0.62
75:3A:501:CDL:H341	75:3A:501:CDL:H211	1.80	0.62
47:3C:299:LEU:CD1	69:3C:512:3PE:H3I3	2.28	0.62
69:3C:512:3PE:H32	69:3C:513:3PE:C22	2.29	0.62
69:3C:513:3PE:H322	69:3C:517:3PE:C31	2.29	0.62
45:3N:444:LEU:HD22	69:3N:503:3PE:C11	2.29	0.62
69:3P:506:3PE:H2F1	69:3P:515:3PE:H371	1.80	0.62
48:3Q:105:ASN:ND2	48:3Q:110:PRO:HD3	2.14	0.62
52:3U:20:VAL:HA	52:3U:23:GLN:HE21	1.64	0.62
54:3X:3:SER:HA	54:3X:6:LEU:HB2	1.81	0.62
7:1G:56:LEU:HD12	7:1G:67:ALA:HA	1.81	0.62
13:1M:442:LEU:HD11	33:1h:25:MET:HE3	1.80	0.62
69:1Y:215:3PE:H261	69:1Y:215:3PE:H362	1.80	0.62
69:1d:201:3PE:C3F	69:1d:201:3PE:C2E	2.77	0.62
34:1i:41:PRO:HA	34:1i:44:GLN:HB2	1.81	0.62
69:1m:204:3PE:H2E2	69:1m:205:3PE:H3C1	1.81	0.62
39:1n:11:HIS:N	45:3N:226:ASP:OD2	2.30	0.62
46:3B:49:LEU:HD23	46:3B:127:THR:HG21	1.80	0.62
47:3C:359:PHE:CD2	69:3C:511:3PE:H3A1	2.34	0.62
69:3Y:107:3PE:H242	69:3Y:107:3PE:C3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
93:4B:303:PSC:H202	63:4I:18:ARG:CG	2.29	0.62
61:4G:62:TRP:CH2	87:4G:103:PEK:H222	2.34	0.62
20:1U:37:MET:HE1	20:1U:44:SER:HA	1.80	0.62
24:1Y:58:TYR:CA	69:1Y:208:3PE:O32	2.41	0.62
24:1Y:107:TYR:HB2	69:1Y:213:3PE:O11	1.98	0.62
24:1Y:122:ALA:CB	70:1Y:202:PC1:C35	2.77	0.62
75:1g:201:CDL:H741	33:1h:30:LEU:O	1.99	0.62
38:1m:26:PRO:HA	38:1m:29:ARG:HG2	1.79	0.62
69:1m:205:3PE:H3A1	69:1m:205:3PE:H3E1	1.82	0.62
51:3G:66:GLN:O	51:3G:70:LYS:HG3	1.99	0.62
55:4A:289:ALA:O	55:4A:291:HIS:N	2.31	0.62
6:1F:151:VAL:HG23	6:1F:154:ARG:HH21	1.64	0.62
7:1G:157:THR:HG22	7:1G:161:ARG:HG3	1.81	0.62
70:1H:403:PC1:H2G2	10:1J:38:GLY:HA3	1.82	0.62
10:1J:88:THR:OG1	69:1J:201:3PE:C3	2.46	0.62
12:1L:575:ILE:HG23	12:1L:579:ASN:ND2	2.14	0.62
50:3F:96:GLU:HG2	50:3F:97:GLU:HG3	1.80	0.62
52:3H:59:ARG:O	52:3H:63:GLU:HG2	2.00	0.62
69:3Q:503:3PE:H2E2	69:3Q:503:3PE:H2I3	1.81	0.62
55:4A:460:ILE:HG12	58:4D:92:THR:HG21	1.80	0.62
59:4E:43:PRO:HB3	59:4E:47:ILE:HD11	1.82	0.62
69:1B:204:3PE:H371	75:1q:202:CDL:H592	1.81	0.62
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	1.81	0.62
7:1G:283:MET:HB3	7:1G:291:LEU:HD22	1.82	0.62
11:1K:93:LEU:HD12	14:1N:54:GLU:HG2	1.80	0.62
14:1N:193:VAL:HG21	14:1N:200:MET:HB2	1.80	0.62
14:1N:242:SER:HB3	69:1N:401:3PE:H241	1.80	0.62
20:1U:8:LEU:N	20:1U:88:GLU:OE2	2.29	0.62
46:3B:95:LYS:HE3	49:3I:72:VAL:HB	1.81	0.62
47:3C:141:TRP:CD1	47:3C:265:PRO:HD3	2.35	0.62
69:3C:509:3PE:H3F2	75:3N:502:CDL:H871	1.81	0.62
45:3N:41:ILE:HG23	45:3N:195:MET:HG3	1.80	0.62
45:3N:329:MET:HE1	51:3T:3:GLU:OE1	1.98	0.62
69:3N:501:3PE:C2A	75:3N:502:CDL:H532	2.29	0.62
1:1A:44:MET:HE3	1:1A:46:SER:N	2.13	0.62
7:1G:194:GLU:HG2	7:1G:195:LEU:HG	1.81	0.62
7:1G:522:LEU:HD22	7:1G:537:LEU:HD21	1.82	0.62
13:1M:98:MET:HE2	13:1M:101:LEU:HD12	1.79	0.62
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.31	0.62
49:3E:213:LEU:HA	49:3E:261:PRO:CD	2.29	0.62
48:3Q:165:TYR:CZ	48:3Q:168:VAL:HG23	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1B:202:PC1:C24	70:1B:202:PC1:H2A1	2.22	0.62
10:1J:7:PHE:HE1	11:1K:3:LEU:HD22	1.64	0.62
10:1J:83:TRP:HZ2	10:1J:93:PHE:CG	2.18	0.62
70:1Y:207:PC1:O32	70:3T:102:PC1:H153	2.00	0.62
29:1d:8:ARG:CD	70:1d:204:PC1:C25	2.77	0.62
69:1d:206:3PE:H371	69:1f:104:3PE:H2B1	1.77	0.62
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.63	0.62
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	1.82	0.62
54:3Y:14:ALA:O	54:3Y:18:ILE:HG13	2.00	0.62
55:4A:289:ALA:HB3	55:4A:305:PHE:CG	2.34	0.62
57:4C:86:PHE:HZ	91:4C:305:PGV:H301	1.65	0.62
12:1L:290:LEU:O	12:1L:523:SER:OG	2.18	0.62
15:1O:296:PHE:CD1	15:1O:299:LEU:HD12	2.34	0.62
69:1Y:201:3PE:H332	51:3T:56:TYR:HD1	1.65	0.62
47:3C:375:ASN:ND2	69:3C:508:3PE:H241	2.15	0.62
69:3P:517:3PE:H3A1	69:3P:518:3PE:C39	2.30	0.62
70:3R:303:PC1:H2G1	70:3X:104:PC1:C2I	2.29	0.62
75:3Y:106:CDL:H622	69:3Y:107:3PE:H272	1.82	0.62
8:1H:65:THR:O	8:1H:124:ASN:ND2	2.29	0.62
69:1Y:215:3PE:C3C	70:3T:102:PC1:H3A2	2.29	0.62
46:3B:435:PHE:HB2	46:3B:438:GLU:CG	2.30	0.62
47:3C:355:SER:CB	69:3C:511:3PE:H372	2.30	0.62
69:3C:509:3PE:H2A1	70:3X:104:PC1:H361	1.82	0.62
47:3P:376:LEU:O	50:3S:17:ARG:HD3	1.99	0.62
69:3P:503:3PE:H3A1	69:3P:503:3PE:H2C2	1.82	0.62
69:3R:304:3PE:H3F2	69:3R:304:3PE:H3B1	1.80	0.62
69:3X:107:3PE:O21	69:3X:107:3PE:C25	2.47	0.62
54:3Y:30:VAL:HG22	69:3Y:105:3PE:H2F1	1.82	0.62
2:1B:175:ILE:O	2:1B:179:ARG:HG3	2.00	0.62
4:1D:94:LYS:HD2	4:1D:102:TYR:HE2	1.65	0.62
12:1L:600:THR:O	12:1L:601:LEU:C	2.43	0.62
14:1N:246:VAL:CG1	69:1N:401:3PE:H2C2	2.29	0.62
25:1Z:97:ILE:HD13	30:1e:82:ARG:HB2	1.81	0.62
75:1q:202:CDL:H562	75:1q:202:CDL:H141	1.82	0.62
46:3B:435:PHE:H	46:3B:438:GLU:HG3	1.65	0.62
47:3C:305:PRO:O	69:3C:506:3PE:C12	2.42	0.62
50:3F:24:TRP:NE1	50:3F:26:GLU:HB2	2.14	0.62
51:3G:56:VAL:HG11	69:3G:109:3PE:H2C1	1.82	0.62
49:3R:175:PHE:HB2	49:3R:213:LEU:O	2.00	0.62
50:3S:12:TRP:HA	50:3S:12:TRP:HE3	1.64	0.62
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:79:ALA:HB2	9:1I:106:THR:HG23	1.82	0.61
70:1Y:207:PC1:H252	69:1Y:209:3PE:H361	1.82	0.61
69:1Y:209:3PE:H11	69:1Y:209:3PE:O22	1.99	0.61
69:3C:511:3PE:H332	69:3C:512:3PE:H282	1.82	0.61
49:3I:64:LEU:HA	49:3I:77:ARG:O	2.00	0.61
46:3O:299:VAL:HG11	46:3O:336:VAL:HG13	1.81	0.61
47:3P:327:MET:CE	70:3T:102:PC1:H3D1	2.29	0.61
54:3X:39:ARG:HG2	54:3X:52:PHE:CZ	2.35	0.61
69:3Y:104:3PE:H321	69:3Y:105:3PE:H271	1.81	0.61
56:4B:7:LEU:HD11	75:4B:302:CDL:H712	1.72	0.61
6:1F:326:GLN:O	6:1F:420:ARG:NH2	2.33	0.61
7:1G:190:MET:HG3	7:1G:192:MET:HG2	1.82	0.61
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.82	0.61
10:1J:65:LEU:O	10:1J:66:VAL:HG23	2.00	0.61
10:1J:175:ASN:H	14:1N:48:PHE:HD2	1.48	0.61
69:1L:711:3PE:H231	69:1M:502:3PE:H231	1.82	0.61
13:1M:341:THR:HG21	38:1m:64:LEU:HD21	1.81	0.61
32:1g:56:TRP:CH2	69:1g:202:3PE:H361	2.35	0.61
38:1m:84:LYS:HG3	69:1m:202:3PE:H11	1.81	0.61
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.82	0.61
49:3I:65:VAL:HG13	49:3I:77:ARG:HH12	1.65	0.61
69:3X:107:3PE:H3D2	69:3X:107:3PE:H3H2	1.82	0.61
55:4A:24:ALA:O	55:4A:28:MET:HG2	2.00	0.61
55:4A:409:TRP:CD1	91:4A:606:PGV:H31	2.34	0.61
6:1F:68:ARG:HD2	6:1F:254:LYS:HZ3	1.65	0.61
8:1H:199:ASP:OD1	8:1H:279:ARG:NE	2.29	0.61
14:1N:21:MET:HE1	69:1e:201:3PE:H3C2	1.80	0.61
15:1O:34:GLY:N	77:1O:401:GTP:O3G	2.34	0.61
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.82	0.61
27:1b:23:ALA:HB1	69:1b:101:3PE:H2G1	1.82	0.61
32:1g:50:ASP:HB3	32:1g:53:VAL:HG22	1.80	0.61
47:3C:4:ILE:HD11	69:3C:515:3PE:O32	2.00	0.61
49:3E:179:ARG:HH21	49:3E:205:VAL:HG21	1.63	0.61
49:3E:254:ALA:HB1	49:3E:255:PRO:HD2	1.82	0.61
49:3R:248:ARG:CD	49:3R:257:ASN:HD22	2.13	0.61
75:3Y:106:CDL:H112	75:3Y:106:CDL:H542	1.81	0.61
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.82	0.61
14:1N:245:MET:CE	69:1N:401:3PE:C38	2.77	0.61
15:1O:230:ASP:OD1	15:1O:230:ASP:N	2.32	0.61
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.33	0.61
17:1Q:88:THR:OG1	17:1Q:91:ASP:OD1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:1Y:217:CDL:OB3	75:1Y:217:CDL:H121	2.00	0.61
47:3C:294:LEU:HD23	47:3C:294:LEU:O	2.00	0.61
51:3G:5:GLU:HB2	51:3G:8:HIS:NE2	2.15	0.61
45:3N:283:THR:HA	46:3O:143:GLN:HE22	1.66	0.61
47:3P:4:ILE:HD11	69:3P:511:3PE:C11	2.23	0.61
69:3W:101:3PE:C3E	69:3W:102:3PE:H261	2.30	0.61
2:1B:92:LEU:HD23	2:1B:133:VAL:HG11	1.82	0.61
2:1B:177:TYR:N	70:1B:202:PC1:H252	2.15	0.61
14:1N:318:GLU:OE2	29:1d:50:ARG:NH1	2.33	0.61
69:1d:201:3PE:H3E1	75:1d:202:CDL:H452	1.81	0.61
35:1j:56:PRO:O	40:1o:106:ARG:NH2	2.33	0.61
43:1r:7:ILE:O	43:1r:11:ARG:HG2	2.00	0.61
69:3N:501:3PE:H292	75:3N:502:CDL:H532	1.83	0.61
69:3N:503:3PE:H2H2	70:3R:303:PC1:H2F2	1.81	0.61
69:3Q:503:3PE:H231	69:3Q:503:3PE:H332	1.82	0.61
54:3Y:33:VAL:HG11	69:3Y:105:3PE:H2H1	1.82	0.61
56:4B:39:LEU:CD2	75:4B:302:CDL:H432	2.31	0.61
75:4B:302:CDL:HA32	75:4B:302:CDL:HB61	1.81	0.61
2:1B:177:TYR:HD1	70:1B:202:PC1:C26	2.13	0.61
75:1H:401:CDL:H512	75:1H:401:CDL:H732	1.82	0.61
69:1L:708:3PE:H31	69:1L:708:3PE:C22	2.31	0.61
13:1M:54:LEU:CD1	33:1h:96:ILE:HD11	2.28	0.61
20:1U:17:TYR:O	20:1U:21:LEU:HD23	2.01	0.61
69:1Y:209:3PE:H381	75:3P:513:CDL:H852	1.82	0.61
46:3B:385:GLN:OE1	46:3B:393:VAL:HG22	2.00	0.61
47:3C:379:TRP:CZ3	50:3F:45:ARG:HD3	2.35	0.61
69:3G:101:3PE:H2C2	69:3G:101:3PE:H2G1	1.82	0.61
69:3P:511:3PE:C2A	69:3P:511:3PE:C2E	2.71	0.61
1:1A:70:ALA:HB2	10:1J:59:ILE:HG12	1.81	0.61
69:1B:204:3PE:H361	69:1B:205:3PE:C3B	2.31	0.61
9:1I:70:TYR:CE2	9:1I:76:ARG:HA	2.36	0.61
14:1N:314:LYS:NZ	15:1O:274:THR:OG1	2.30	0.61
15:1O:73:LEU:HD21	15:1O:295:LYS:HB3	1.83	0.61
69:1d:206:3PE:C38	69:1f:104:3PE:H292	2.31	0.61
32:1g:108:MET:HG3	41:1p:134:VAL:HG13	1.81	0.61
49:3E:182:LYS:HD3	49:3E:183:GLU:HG2	1.83	0.61
46:3O:213:HIS:O	46:3O:217:LYS:HG3	2.01	0.61
52:3U:20:VAL:HG12	52:3U:69:VAL:HG22	1.81	0.61
55:4A:508:PRO:HG3	57:4C:6:HIS:HB3	1.82	0.61
91:4A:609:PGV:C25	66:4L:28:TYR:HB3	2.30	0.61
4:1D:249:ASP:OD2	4:1D:404:LYS:NZ	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:262:VAL:HG23	6:1F:336:VAL:HG21	1.82	0.61
75:1L:704:CDL:H181	69:1L:709:3PE:H241	1.81	0.61
24:1Y:108:GLY:C	70:1Y:206:PC1:H31	2.25	0.61
47:3C:352:GLN:HE21	69:3C:511:3PE:C22	2.08	0.61
75:3F:201:CDL:H831	75:3F:201:CDL:H612	1.83	0.61
46:3O:69:LEU:HD13	46:3O:105:MET:HE1	1.83	0.61
47:3P:28:SER:HB2	75:3P:513:CDL:OA4	2.01	0.61
69:3P:510:3PE:H3C2	69:3P:517:3PE:C2I	2.30	0.61
10:1J:92:ALA:HB1	69:1J:203:3PE:H332	1.82	0.61
13:1M:10:MET:HE2	69:1f:104:3PE:C38	2.27	0.61
20:1T:25:ILE:HG23	20:1T:40:LEU:HD22	1.83	0.61
31:1f:11:TRP:HB2	69:1f:101:3PE:H2B1	1.83	0.61
47:3C:126:THR:HG21	47:3C:186:PRO:HG3	1.82	0.61
49:3E:228:ALA:HA	49:3E:232:GLY:HA2	1.83	0.61
69:3Q:502:3PE:H231	69:3Q:502:3PE:H341	1.83	0.61
54:3X:44:TRP:CE3	69:3X:108:3PE:H372	2.34	0.61
1:1A:104:TYR:HB2	69:1A:203:3PE:C37	2.31	0.61
15:1O:34:GLY:HA2	15:1O:37:ARG:NH1	2.16	0.61
16:1P:97:ARG:NH2	79:1P:501:NDP:O1A	2.31	0.61
31:1f:56:TRP:HE1	33:1h:88:GLU:HG3	1.66	0.61
47:3C:287:LYS:HD2	69:3C:513:3PE:HN2	1.64	0.61
49:3E:231:PHE:HE1	49:3E:242:HIS:HB3	1.65	0.61
53:3J:46:HIS:CD2	69:3J:101:3PE:H342	2.36	0.61
45:3N:17:SER:HB2	45:3N:209:LEU:CD1	2.31	0.61
46:3O:65:THR:HA	46:3O:186:VAL:HG11	1.82	0.61
69:3P:506:3PE:C3I	69:3P:517:3PE:H371	2.30	0.61
49:3R:170:ARG:C	49:3R:172:LYS:H	2.09	0.61
69:3W:102:3PE:H32	69:3W:102:3PE:O22	2.00	0.61
91:4A:609:PGV:H252	66:4L:28:TYR:CB	2.30	0.61
75:4B:302:CDL:H472	75:4B:302:CDL:H431	1.81	0.61
57:4C:54:MET:HE3	57:4C:58:TRP:HZ3	1.65	0.61
2:1B:116:MET:HE3	2:1B:156:LEU:HB2	1.82	0.60
2:1B:177:TYR:CD1	70:1B:202:PC1:C26	2.84	0.60
7:1G:213:TYR:HE1	7:1G:248:MET:HB3	1.66	0.60
8:1H:96:ILE:CG2	25:1Z:144:THR:HB	2.31	0.60
69:1J:201:3PE:H2B1	69:1Y:210:3PE:C34	2.31	0.60
69:1N:401:3PE:H2C1	69:1N:401:3PE:C3E	2.30	0.60
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.36	0.60
45:3A:156:THR:HB	45:3A:241:ILE:HG13	1.81	0.60
75:3A:501:CDL:H201	69:3A:503:3PE:H3B2	1.82	0.60
47:3C:342:PRO:HB2	47:3C:344:GLU:HG2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:377:LEU:HG	50:3F:32:TYR:CE2	2.34	0.60
52:3U:28:GLU:HA	52:3U:31:ILE:HB	1.83	0.60
91:4A:607:PGV:H31	75:4C:306:CDL:H462	1.83	0.60
57:4C:160:ILE:HG22	91:4C:302:PGV:H91	1.83	0.60
63:4I:22:VAL:O	63:4I:26:ILE:HG13	2.01	0.60
8:1H:244:GLY:O	70:1H:404:PC1:H143	2.01	0.60
12:1L:429:PHE:O	12:1L:436:ARG:NH2	2.34	0.60
69:1Y:201:3PE:H282	69:1Y:214:3PE:H2A1	1.81	0.60
29:1d:10:PRO:HA	70:1d:204:PC1:H221	1.82	0.60
34:1i:52:ASP:HB3	34:1i:57:LYS:HE3	1.82	0.60
38:1m:92:PHE:CG	69:1m:203:3PE:C27	2.84	0.60
75:1q:202:CDL:H272	75:1q:202:CDL:H441	1.84	0.60
69:3C:516:3PE:H392	69:3C:516:3PE:H292	1.83	0.60
52:3H:42:LEU:HD13	52:3H:98:LEU:HD22	1.82	0.60
69:3N:501:3PE:H281	75:3N:502:CDL:H512	1.82	0.60
69:3N:501:3PE:H271	75:3X:103:CDL:H651	1.83	0.60
46:3O:43:PRO:O	46:3O:113:ARG:HG3	2.00	0.60
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.65	0.60
75:1H:401:CDL:H732	75:1H:401:CDL:C51	2.32	0.60
76:1I:203:AYA:HM2	42:1q:58:ARG:HD3	1.82	0.60
13:1M:54:LEU:HD23	33:1h:93:ILE:HG23	1.83	0.60
70:1M:501:PC1:C11	75:1i:201:CDL:H112	2.31	0.60
24:1Y:95:ALA:CB	70:1Y:207:PC1:H3C1	2.28	0.60
69:1Y:205:3PE:H261	69:1Y:205:3PE:H2A2	1.81	0.60
27:1b:27:LEU:HD11	69:1b:101:3PE:C2G	2.32	0.60
32:1g:70:LEU:O	32:1g:74:SER:OG	2.18	0.60
45:3A:305:GLN:HE22	49:3I:42:VAL:HG12	1.66	0.60
75:3N:502:CDL:H341	75:3N:502:CDL:H201	1.83	0.60
48:3Q:33:TYR:HA	48:3Q:37:CYS:SG	2.40	0.60
91:4A:608:PGV:H343	75:4B:302:CDL:H873	1.82	0.60
57:4C:98:PHE:HB2	91:4C:303:PGV:H102	1.82	0.60
2:1B:144:ILE:HD12	2:1B:162:GLN:HG2	1.83	0.60
6:1F:15:LEU:HD13	6:1F:271:GLU:HB2	1.84	0.60
8:1H:91:MET:O	8:1H:93:TYR:N	2.33	0.60
12:1L:546:GLN:HA	12:1L:550:SER:HB3	1.82	0.60
24:1Y:27:ILE:CG2	69:1Y:208:3PE:H2F2	2.30	0.60
75:1g:201:CDL:H711	33:1h:27:PHE:HD1	1.66	0.60
69:1l:202:3PE:H121	69:1m:204:3PE:O32	2.02	0.60
49:3E:234:TYR:HD2	49:3E:247:GLY:HA2	1.65	0.60
93:4B:303:PSC:H071	59:4E:40:ASP:OD2	2.02	0.60
91:4C:303:PGV:H151	91:4N:101:PGV:H312	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:361:GLN:NE2	17:1Q:133:LYS:HZ3	1.99	0.60
13:1M:94:LEU:HD21	69:1N:401:3PE:H232	1.82	0.60
15:1O:105:LEU:HD11	15:1O:163:TYR:CE2	2.37	0.60
39:1n:58:LYS:HD3	39:1n:58:LYS:H	1.65	0.60
69:3C:511:3PE:H2D1	69:3C:511:3PE:H291	1.83	0.60
49:3E:220:LEU:HD12	47:3P:263:ASN:HD21	1.64	0.60
46:3O:163:LEU:HD11	46:3O:258:VAL:HG22	1.82	0.60
50:3S:12:TRP:NE1	50:3S:14:GLU:HB2	2.16	0.60
1:1A:108:GLN:NE2	69:1A:203:3PE:C24	2.65	0.60
69:1B:205:3PE:H322	75:1q:202:CDL:H781	1.83	0.60
4:1D:52:GLY:N	4:1D:53:PRO:HD3	2.15	0.60
12:1L:463:PHE:CB	69:1L:703:3PE:C27	2.78	0.60
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.34	0.60
23:1X:166:LEU:O	23:1X:169:TRP:HE3	1.84	0.60
34:1i:18:ARG:NH1	39:1n:170:VAL:O	2.35	0.60
35:1j:38:TRP:CD1	69:1k:101:3PE:H382	2.31	0.60
45:3A:395:TRP:O	45:3A:399:ILE:HG13	2.02	0.60
69:3A:502:3PE:H3C1	69:3E:303:3PE:H3E1	1.82	0.60
48:3Q:222:MET:HE2	49:3R:121:THR:HG21	1.84	0.60
53:3W:35:ALA:HB1	69:3W:102:3PE:H251	1.83	0.60
12:1L:602:PHE:HB3	12:1L:604:TYR:CZ	2.37	0.60
49:3E:173:PRO:O	49:3E:215:GLY:N	2.33	0.60
51:3G:67:GLU:OE2	69:3G:110:3PE:H122	2.01	0.60
47:3P:142:GLY:O	47:3P:146:ILE:HG23	2.02	0.60
48:3Q:156:GLN:HG2	52:3U:59:PHE:CZ	2.36	0.60
49:3R:235:TYR:HB2	49:3R:242:HIS:CB	2.32	0.60
51:3T:64:GLN:O	51:3T:68:LYS:HG3	2.00	0.60
55:4A:423:MET:CE	91:4K:101:PGV:H341	2.31	0.60
3:1C:173:GLU:HG3	3:1C:188:VAL:HA	1.83	0.60
7:1G:320:GLY:O	7:1G:498:SER:OG	2.20	0.60
11:1K:94:ASN:ND2	12:1L:581:LYS:O	2.30	0.60
12:1L:534:HIS:HB3	69:1L:701:3PE:O14	2.01	0.60
69:1N:401:3PE:C2F	69:1d:201:3PE:H2I2	2.32	0.60
69:1Y:205:3PE:H272	69:1Y:208:3PE:H272	1.84	0.60
69:3C:515:3PE:H2	69:3C:516:3PE:H222	1.83	0.60
49:3E:152:ILE:HA	49:3E:169:TRP:HZ3	1.65	0.60
45:3N:204:GLU:HB3	45:3N:207[B]:GLN:HG2	1.82	0.60
70:3X:104:PC1:H382	69:3X:107:3PE:H3H1	1.84	0.60
54:3Y:44:TRP:CB	69:3Y:105:3PE:H3A2	2.30	0.60
55:4A:415:VAL:HG22	91:4A:608:PGV:H62	1.83	0.60
91:4A:609:PGV:H202	66:4L:28:TYR:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:628:PRO:HD2	19:1S:55:ARG:HB3	1.83	0.60
10:1J:46:ASN:ND2	25:1Z:142:TRP:HE1	2.00	0.60
12:1L:260:LEU:HG	12:1L:267:MET:HE1	1.84	0.60
45:3A:192:ALA:H	45:3A:220:SER:HG	1.48	0.60
69:3P:508:3PE:C2G	69:3P:519:3PE:H3G2	2.30	0.60
55:4A:423:MET:HE1	91:4K:101:PGV:H341	1.84	0.60
75:4B:302:CDL:H151	75:4B:302:CDL:H191	1.83	0.60
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	1.83	0.60
14:1N:245:MET:O	14:1N:249:LEU:HG	2.01	0.60
69:1N:401:3PE:H221	69:1d:201:3PE:C31	2.32	0.60
15:1O:53:GLU:HG3	15:1O:125:GLU:O	2.02	0.60
75:3A:501:CDL:H631	69:3A:502:3PE:H2I1	1.83	0.60
69:3C:513:3PE:H322	69:3C:517:3PE:H32	1.84	0.60
45:3N:241:ILE:HD11	49:3R:83:ILE:HD11	1.84	0.60
47:3P:10:LEU:CD2	69:3P:512:3PE:C38	2.69	0.60
47:3P:138:MET:HE1	47:3P:268:ILE:HA	1.83	0.60
48:3Q:30:PHE:CE2	48:3Q:34:LYS:HD2	2.37	0.60
49:3R:219:HIS:CE1	49:3R:253:PRO:HG2	2.37	0.60
54:3X:44:TRP:CE3	69:3X:108:3PE:C37	2.85	0.60
55:4A:102:PHE:CZ	91:4A:609:PGV:H91	2.35	0.60
75:4C:306:CDL:H541	75:4C:306:CDL:H132	1.84	0.60
5:1E:184:PRO:HG2	44:1s:44:HIS:HD2	1.67	0.59
9:1I:53:GLU:HG2	42:1q:61:TRP:HB3	1.83	0.59
12:1L:464:ALA:HB2	69:1L:703:3PE:H2C1	1.84	0.59
13:1M:6:ILE:HD12	31:1f:23:GLY:CA	2.31	0.59
13:1M:6:ILE:HD11	31:1f:26:LEU:HD12	1.83	0.59
13:1M:190:TRP:HZ3	69:1m:201:3PE:H342	1.66	0.59
17:1Q:23:THR:HG23	17:1Q:25:VAL:HG23	1.84	0.59
24:1Y:102:ALA:HB2	70:1Y:207:PC1:H2	1.84	0.59
75:1Y:217:CDL:H162	51:3T:46:LEU:HD13	1.84	0.59
69:1Z:201:3PE:H2C2	69:1Z:201:3PE:H3B1	1.83	0.59
69:1Z:201:3PE:H222	43:1r:13:TRP:CZ2	2.38	0.59
32:1g:56:TRP:CE2	69:1g:202:3PE:H331	2.37	0.59
38:1m:99:PHE:CE2	69:1m:205:3PE:C3G	2.70	0.59
45:3A:241:ILE:HD11	49:3E:85:VAL:HG22	1.82	0.59
46:3B:78:LYS:HB2	46:3B:129:ALA:HB1	1.84	0.59
45:3N:214:LYS:HG3	45:3N:215:HIS:CD2	2.37	0.59
47:3P:128:PHE:CE1	47:3P:146:ILE:HG12	2.36	0.59
47:3P:234:PHE:CE2	75:3T:101:CDL:H532	2.37	0.59
49:3R:93:ARG:HD3	69:3R:305:3PE:H122	1.84	0.59
56:4B:61:VAL:HG13	93:4B:303:PSC:H271	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4C:98:PHE:CE1	57:4C:252:LEU:HD12	2.37	0.59
13:1M:16:TRP:HA	13:1M:93:LYS:HD3	1.83	0.59
69:1M:502:3PE:H261	69:1l:204:3PE:H381	1.83	0.59
14:1N:336:VAL:HG21	69:1d:203:3PE:H2H2	1.84	0.59
69:1Y:205:3PE:H321	70:1Y:206:PC1:H382	1.84	0.59
75:1d:202:CDL:OB9	69:1f:104:3PE:H262	2.02	0.59
45:3A:368:HIS:O	45:3A:370:ASP:N	2.32	0.59
47:3C:323:CYS:O	47:3C:327:MET:HG3	2.02	0.59
48:3D:115:ARG:O	48:3D:119:GLN:HG3	2.02	0.59
69:3D:503:3PE:H3G2	69:3G:101:3PE:H2B1	1.83	0.59
75:3F:201:CDL:H172	69:3G:109:3PE:H342	1.84	0.59
69:3G:108:3PE:H251	69:3G:108:3PE:C34	2.29	0.59
45:3N:127:ILE:O	45:3N:131:ARG:HG3	2.02	0.59
69:3Q:503:3PE:C36	69:3W:101:3PE:H341	2.32	0.59
49:3R:182:LYS:HD3	49:3R:182:LYS:H	1.66	0.59
49:3R:236:CYS:SG	72:3R:301:FES:S2	2.99	0.59
69:3W:102:3PE:H351	69:3W:102:3PE:H232	1.84	0.59
55:4A:21:LEU:HD13	91:4A:609:PGV:C6	2.32	0.59
57:4C:102:TYR:HB2	91:4C:303:PGV:H51	1.83	0.59
1:1A:23:TRP:HA	70:1A:202:PC1:C12	2.31	0.59
7:1G:36:GLN:NE2	17:1Q:47:SER:O	2.35	0.59
13:1M:1:FME:HG3	13:1M:52:PHE:CD2	2.38	0.59
15:1O:101:TYR:HE1	15:1O:128:ILE:HG23	1.66	0.59
75:1Y:217:CDL:H181	70:3T:102:PC1:O32	2.03	0.59
45:3A:241:ILE:HD11	49:3E:85:VAL:CG2	2.32	0.59
46:3B:118:ILE:O	46:3B:121:GLU:HG2	2.02	0.59
48:3D:232:ARG:NE	48:3D:233:GLU:O	2.35	0.59
49:3E:183:GLU:O	49:3E:187:GLU:HG2	2.02	0.59
51:3G:44:ARG:HH22	69:3G:105:3PE:H122	1.56	0.59
75:3P:513:CDL:C63	75:3T:101:CDL:C34	2.76	0.59
49:3R:234:TYR:HD2	49:3R:243:TYR:CB	2.14	0.59
69:3S:201:3PE:H341	69:3S:201:3PE:H282	1.84	0.59
69:3W:103:3PE:H3H2	69:3X:101:3PE:H3G2	1.84	0.59
75:3Y:106:CDL:H522	75:3Y:106:CDL:HB4	1.85	0.59
55:4A:96:ARG:HE	57:4C:11:VAL:HG11	1.67	0.59
68:4N:40:ASN:HB3	68:4N:43:VAL:CG2	2.32	0.59
1:1A:27:LEU:HD22	70:1A:202:PC1:C15	2.32	0.59
5:1E:36:LYS:O	44:1s:65:GLN:NE2	2.36	0.59
8:1H:228:TYR:HA	8:1H:231:ILE:HD12	1.83	0.59
10:1J:96:GLY:HA3	69:1J:203:3PE:H391	1.83	0.59
10:1J:151:THR:HG21	70:1J:202:PC1:H32	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:99:TRP:CD2	16:1P:277:PRO:HD2	2.37	0.59
70:1Y:207:PC1:O14	70:1Y:207:PC1:H152	2.02	0.59
69:1Y:210:3PE:H2B1	75:1Y:217:CDL:H852	1.83	0.59
75:1g:201:CDL:OB4	33:1h:23:LYS:HD2	2.02	0.59
34:1i:13:GLN:HE22	39:1n:156:ALA:HB3	1.66	0.59
47:3C:296:ALA:CB	69:3C:511:3PE:C3G	2.79	0.59
69:3C:505:3PE:H111	69:3C:505:3PE:H31	1.83	0.59
48:3D:232:ARG:HH11	49:3R:237:PRO:CB	2.13	0.59
49:3R:159:ILE:HD13	49:3R:176:VAL:HG11	1.85	0.59
49:3R:225:ILE:HG22	49:3R:228:ALA:HB3	1.85	0.59
57:4C:25:LEU:HD23	64:4J:43:THR:HG22	1.84	0.59
6:1F:405:CYS:HG	71:1F:502:SF4:FE2	1.15	0.59
10:1J:99:MET:HE2	69:1J:201:3PE:H3F1	1.78	0.59
10:1J:143:ILE:HG13	11:1K:57:ASN:HB3	1.84	0.59
13:1M:25:ILE:HG23	32:1g:60:VAL:HG21	1.83	0.59
16:1P:99:TRP:CG	16:1P:277:PRO:HD2	2.38	0.59
24:1Y:80:ARG:HH11	69:1Y:212:3PE:C22	2.15	0.59
69:1Y:201:3PE:H371	51:3T:56:TYR:HB2	1.84	0.59
69:3G:107:3PE:H241	69:3G:107:3PE:H281	1.83	0.59
53:3J:23:LEU:HD23	69:3J:103:3PE:H3A2	1.83	0.59
52:3U:32:LYS:O	52:3U:35:GLU:HG2	2.02	0.59
57:4C:148:HIS:O	57:4C:152:MET:HG3	2.02	0.59
1:1A:103:ALA:HB1	69:1b:101:3PE:H321	1.83	0.59
4:1D:151:ILE:HG12	4:1D:170:MET:HE3	1.84	0.59
6:1F:197:GLU:OE1	6:1F:204:ARG:NH2	2.35	0.59
6:1F:362:CYS:SG	71:1F:502:SF4:S3	3.01	0.59
70:1H:402:PC1:H3F1	27:1b:24:ILE:HD12	1.84	0.59
70:1H:404:PC1:H3I1	69:1Z:201:3PE:C27	2.33	0.59
12:1L:55:MET:CE	69:1o:201:3PE:H2I3	2.33	0.59
16:1P:236:TYR:HB2	16:1P:241:LEU:HD22	1.84	0.59
38:1m:92:PHE:HE1	69:1m:203:3PE:H362	1.61	0.59
40:1o:102:GLU:OE2	40:1o:105:ARG:NH1	2.36	0.59
47:3C:121:PHE:HA	47:3C:124:MET:HE3	1.84	0.59
69:3C:511:3PE:H321	69:3C:512:3PE:H262	1.84	0.59
69:3C:515:3PE:H32	69:3C:516:3PE:O32	2.03	0.59
48:3D:163:ASN:ND2	48:3D:164:GLU:H	2.00	0.59
75:3N:502:CDL:H611	69:3P:511:3PE:H2F1	1.84	0.59
47:3P:8:HIS:HD2	47:3P:11:MET:H	1.50	0.59
47:3P:152:ALA:HB2	47:3P:287:LYS:HD2	1.84	0.59
47:3P:375:ASN:HB3	69:3P:516:3PE:C3	2.32	0.59
75:3X:103:CDL:H211	69:3X:105:3PE:H3H2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.03	0.59
5:1E:105:THR:OG1	72:1E:301:FES:S2	2.61	0.59
8:1H:173:TRP:CB	8:1H:175:ILE:HG22	2.32	0.59
10:1J:39:VAL:O	10:1J:43:ILE:HG13	2.02	0.59
11:1K:73:LEU:HD21	14:1N:41:ILE:HG13	1.84	0.59
13:1M:153:THR:CG2	13:1M:206:LYS:HZ3	2.15	0.59
69:1Y:215:3PE:H2B2	69:1Y:215:3PE:H371	1.84	0.59
69:1Y:215:3PE:H3A1	69:3P:517:3PE:H2H1	1.85	0.59
29:1d:54:VAL:HG11	69:1f:101:3PE:H12	1.85	0.59
42:1q:34:ARG:HD2	42:1q:54:GLN:HE22	1.67	0.59
47:3C:29:SER:HA	47:3C:32:ASN:HD22	1.66	0.59
69:3C:515:3PE:H351	69:3C:515:3PE:H2B1	1.84	0.59
69:3N:501:3PE:O32	69:3P:511:3PE:H322	2.01	0.59
49:3R:246:SER:O	49:3R:247:GLY:C	2.46	0.59
69:3T:103:3PE:H11	69:3T:103:3PE:HN2	1.66	0.59
53:3W:21:PHE:O	53:3W:25:ILE:HD12	2.03	0.59
69:3W:102:3PE:H361	69:3X:101:3PE:C34	2.33	0.59
12:1L:460:GLY:HA2	69:1L:703:3PE:H2B1	1.84	0.59
69:1L:706:3PE:P	14:1N:152:ASN:HD22	2.26	0.59
38:1m:29:ARG:HA	39:1n:8:TYR:OH	2.03	0.59
40:1o:55:ARG:HH22	41:1p:119:SER:HB3	1.67	0.59
48:3D:125:CYS:SG	86:3D:501:HEC:HBB3	2.42	0.59
85:3P:501:HEM:HBC2	85:3P:501:HEM:HMC1	1.85	0.59
49:3R:93:ARG:NH2	51:3T:21:PHE:HA	2.17	0.59
49:3R:232:GLY:CA	49:3R:244:ASP:HA	2.27	0.59
6:1F:101:GLU:HG3	6:1F:184:TYR:HE1	1.67	0.59
12:1L:534:HIS:CB	69:1L:701:3PE:O14	2.51	0.59
69:1L:709:3PE:H251	69:1L:709:3PE:C32	2.32	0.59
24:1Y:22:TYR:CE1	75:1Y:217:CDL:H471	2.38	0.59
24:1Y:75:ILE:CG2	69:1Y:214:3PE:C26	2.80	0.59
69:1Y:209:3PE:C3C	69:1Y:212:3PE:H2E1	2.32	0.59
45:3A:51:LYS:HG3	45:3A:52:ASN:N	2.18	0.59
45:3A:398:ARG:O	45:3A:401:GLU:HG2	2.01	0.59
46:3O:166:ALA:O	46:3O:240:ARG:HG3	2.03	0.59
47:3P:221:HIS:O	47:3P:222:PRO:C	2.43	0.59
49:3R:241:SER:HB3	49:3R:249:ILE:HD12	1.85	0.59
55:4A:1:FME:O1	91:4A:609:PGV:O05	1.87	0.59
68:4N:32:TYR:O	68:4N:33:VAL:HB	2.02	0.59
13:1M:40:SER:HB3	70:1h:203:PC1:C33	2.32	0.59
29:1d:8:ARG:CD	70:1d:204:PC1:C24	2.81	0.59
70:1h:202:PC1:H11	41:1p:60:TYR:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3D:303:LEU:HD12	69:3D:503:3PE:H382	1.85	0.59
69:3P:517:3PE:H3B2	69:3P:518:3PE:H2F1	1.84	0.59
48:3Q:41:HIS:HE1	48:3Q:111:PRO:HD2	1.68	0.59
48:3Q:105:ASN:HD21	48:3Q:110:PRO:HD3	1.66	0.59
48:3Q:212:MET:HE2	69:3R:302:3PE:H352	1.85	0.59
87:3X:102:PEK:HN2	60:4F:1:ALA:HB1	1.64	0.59
54:3Y:9:ARG:HH12	75:3Y:106:CDL:HB21	1.68	0.59
54:3Y:30:VAL:HA	69:3Y:105:3PE:H2G2	1.85	0.59
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.85	0.58
7:1G:594:ARG:NH1	22:1W:122:PHE:O	2.36	0.58
7:1G:668:ILE:H	7:1G:668:ILE:HD12	1.68	0.58
70:1H:403:PC1:H372	10:1J:57:PHE:CZ	2.38	0.58
10:1J:87:LYS:HB3	69:1J:201:3PE:O14	2.03	0.58
12:1L:208:CYS:HA	69:1L:711:3PE:H112	1.85	0.58
12:1L:602:PHE:CD2	69:1L:706:3PE:O32	2.53	0.58
14:1N:325:LEU:O	14:1N:329:MET:HG2	2.02	0.58
15:1O:27:VAL:HG23	15:1O:125:GLU:HA	1.85	0.58
15:1O:76:ASN:O	15:1O:95:ARG:NE	2.30	0.58
16:1P:267:GLY:O	16:1P:271:GLU:HG3	2.03	0.58
24:1Y:132:TRP:CZ3	82:1Y:203:PGT:H151	2.39	0.58
75:1q:202:CDL:H821	75:1q:202:CDL:H331	1.85	0.58
47:3C:356:ILE:HG23	69:3C:512:3PE:H2E1	1.85	0.58
69:3C:509:3PE:H251	69:3X:107:3PE:H3B2	1.84	0.58
48:3D:186:PRO:O	48:3D:190:ARG:HG3	2.02	0.58
49:3E:263:TYR:CG	49:3E:271:VAL:HB	2.37	0.58
50:3F:114:LYS:O	50:3F:118:GLU:HG2	2.03	0.58
49:3I:41:PRO:HB2	49:3I:44:ASP:CB	2.33	0.58
47:3P:315:MET:HE1	47:3P:325:PHE:CB	2.33	0.58
49:3R:235:TYR:O	49:3R:237:PRO:HD3	2.02	0.58
69:3W:102:3PE:H331	69:3X:101:3PE:H341	1.85	0.58
54:3X:8:PRO:O	54:3X:12:GLU:HG3	2.02	0.58
69:3Y:101:3PE:H381	69:3Y:101:3PE:H2B2	1.85	0.58
3:1C:33:LEU:HD13	3:1C:60:VAL:HG22	1.85	0.58
7:1G:192:MET:HG3	7:1G:691:VAL:HG22	1.86	0.58
14:1N:325:LEU:CA	75:1d:205:CDL:OA4	2.51	0.58
16:1P:27:THR:HG21	16:1P:56:THR:HG22	1.85	0.58
23:1X:136:LEU:HD23	23:1X:137:PRO:HD2	1.85	0.58
30:1e:27:LYS:NZ	33:1h:134:ASP:OD2	2.36	0.58
69:1f:102:3PE:H282	69:1g:202:3PE:H2B2	1.84	0.58
45:3N:17:SER:HB2	45:3N:209:LEU:HD11	1.83	0.58
46:3O:109:VAL:HB	46:3O:119:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:3Y:10:TYR:HB3	75:3Y:106:CDL:H351	1.85	0.58
54:3Y:33:VAL:CG1	69:3Y:105:3PE:H2H1	2.33	0.58
54:3Y:39:ARG:HA	54:3Y:42:LEU:HB2	1.84	0.58
61:4G:68:THR:HG22	61:4G:69:LEU:H	1.68	0.58
24:1Y:140:VAL:O	33:1h:115:ARG:NH1	2.36	0.58
49:3E:178:HIS:HA	49:3E:210:TRP:CD1	2.38	0.58
47:3P:227:LYS:HE2	75:3T:101:CDL:HB62	1.85	0.58
47:3P:278:TYR:CZ	47:3P:282:ARG:HD3	2.38	0.58
47:3P:278:TYR:CE2	47:3P:282:ARG:HD3	2.38	0.58
49:3R:152:ILE:HA	49:3R:274:GLY:HA2	1.86	0.58
69:1J:201:3PE:H2A2	69:1J:201:3PE:H3A1	1.84	0.58
12:1L:214:ILE:HG21	69:1L:711:3PE:H371	1.86	0.58
12:1L:296:ASN:H	39:1n:77:GLN:HE22	1.52	0.58
18:1R:38:ASN:HB3	18:1R:43:LEU:HD11	1.84	0.58
21:1V:34:LEU:HD13	21:1V:48:GLU:HG2	1.86	0.58
22:1W:49:LEU:HD21	22:1W:96:VAL:HG22	1.86	0.58
31:1f:53:GLU:HG2	31:1f:54:VAL:HG22	1.85	0.58
47:3C:168:PHE:CZ	49:3R:151:LYS:HD3	2.39	0.58
47:3C:221:HIS:HA	47:3C:225:THR:HG23	1.86	0.58
49:3E:206:LYS:HD2	49:3E:265:PHE:HD1	1.67	0.58
69:3W:101:3PE:C27	69:3W:102:3PE:H221	2.33	0.58
54:3X:11:ARG:HB3	54:3X:15:ARG:HH21	1.68	0.58
4:1D:246:THR:HB	4:1D:249:ASP:HB2	1.85	0.58
7:1G:579:ARG:HG2	7:1G:636:VAL:HB	1.84	0.58
8:1H:179:TRP:N	8:1H:180:PRO:HD2	2.19	0.58
70:1H:403:PC1:H132	25:1Z:144:THR:HG22	1.83	0.58
9:1I:54:LYS:HD3	42:1q:91:HIS:CE1	2.39	0.58
15:1O:176:VAL:HA	15:1O:179:ILE:HD12	1.85	0.58
16:1P:201:VAL:HG12	16:1P:290:SER:HB3	1.85	0.58
24:1Y:113:ALA:HA	70:1Y:206:PC1:H372	1.84	0.58
69:1Y:201:3PE:H331	69:1Y:201:3PE:H31	1.86	0.58
31:1f:16:VAL:HG12	69:1f:103:3PE:H3F2	1.84	0.58
47:3C:299:LEU:CD1	69:3C:512:3PE:H3I1	2.33	0.58
48:3D:151:ALA:O	48:3D:155:GLU:HG3	2.04	0.58
45:3N:209:LEU:O	45:3N:213:GLN:HG3	2.04	0.58
46:3O:219:VAL:HA	46:3O:222:ARG:HG2	1.84	0.58
49:3R:205:VAL:HG23	49:3R:210:TRP:O	2.03	0.58
49:3R:256:LEU:HG	49:3R:257:ASN:O	2.03	0.58
54:3X:9:ARG:NH1	54:3X:13:LEU:HD11	2.19	0.58
55:4A:418:PHE:CE2	91:4A:608:PGV:H101	2.38	0.58
91:4C:304:PGV:H31	61:4G:70:PHE:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:383:ASN:ND2	7:1G:665:GLN:O	2.35	0.58
75:1L:704:CDL:C59	13:1M:371:PRO:HD2	2.32	0.58
14:1N:218:LEU:HD22	14:1N:240:ILE:HG23	1.85	0.58
15:1O:27:VAL:CG2	15:1O:125:GLU:HA	2.34	0.58
17:1Q:69:LEU:HG	17:1Q:70:MET:HG2	1.86	0.58
75:1d:202:CDL:H391	69:1f:104:3PE:H2E1	1.84	0.58
31:1f:21:VAL:HG12	69:1f:103:3PE:H361	1.84	0.58
40:1o:30:PHE:HB2	40:1o:33:ARG:HD3	1.85	0.58
75:1q:201:CDL:H162	75:1q:201:CDL:C33	2.33	0.58
45:3A:302:LYS:N	45:3A:302:LYS:HD2	2.19	0.58
69:3C:508:3PE:H392	69:3C:508:3PE:H2B2	1.84	0.58
69:3P:515:3PE:H2F1	70:3T:102:PC1:H2D2	1.84	0.58
48:3Q:178:THR:HG22	52:3U:13:LEU:HG	1.86	0.58
54:3X:47:TYR:HA	69:3X:101:3PE:C3	2.29	0.58
61:4G:68:THR:HB	87:4G:103:PEK:O14	2.04	0.58
68:4N:2:LEU:H	68:4N:2:LEU:HD12	1.64	0.58
8:1H:104:PHE:O	8:1H:108:MET:HG2	2.04	0.58
12:1L:127:THR:HA	12:1L:130:ILE:HD12	1.84	0.58
69:1Y:210:3PE:H351	69:1Y:210:3PE:O32	2.04	0.58
29:1d:8:ARG:HD3	70:1d:204:PC1:C24	2.34	0.58
49:3E:217:CYS:HB2	49:3E:224:PRO:HG3	1.85	0.58
49:3E:223:VAL:HB	49:3E:238:CYS:HB2	1.85	0.58
49:3E:270:LEU:O	49:3E:271:VAL:HG22	2.02	0.58
52:3H:53:GLU:HG3	52:3H:57:LYS:HG2	1.86	0.58
45:3N:145:MET:HA	45:3N:148:VAL:CG1	2.33	0.58
46:3O:359:ALA:O	46:3O:363:LYS:HG3	2.04	0.58
47:3P:337:TRP:O	47:3P:341:GLN:HG2	2.02	0.58
47:3P:361:ILE:HG12	47:3P:365:LEU:HD12	1.84	0.58
69:3Q:503:3PE:C3D	69:3W:101:3PE:H2C1	2.33	0.58
49:3R:159:ILE:HA	49:3R:165:MET:HG3	1.86	0.58
49:3R:174:LEU:HD11	49:3R:212:ILE:HG23	1.85	0.58
49:3R:204:ARG:HH22	49:3R:213:LEU:HD23	1.68	0.58
49:3R:263:TYR:O	49:3R:263:TYR:HD1	1.86	0.58
91:4A:606:PGV:H211	91:4A:606:PGV:H61	1.83	0.58
2:1B:90:GLY:HA2	71:1B:201:SF4:S2	2.44	0.58
70:1H:403:PC1:H2F2	10:1J:39:VAL:HG13	1.86	0.58
75:1L:704:CDL:H622	13:1M:448:THR:CG2	2.31	0.58
15:1O:27:VAL:HG21	15:1O:39:ALA:HB2	1.86	0.58
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.68	0.58
20:1U:16:LEU:HD21	20:1U:32:VAL:HA	1.86	0.58
24:1Y:75:ILE:HG21	69:1Y:214:3PE:C28	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:34:LYS:HZ1	64:4J:17:ASP:CG	2.08	0.58
46:3B:200:THR:CB	46:3B:227:ARG:HG2	2.27	0.58
47:3C:356:ILE:HA	69:3C:511:3PE:H391	1.86	0.58
69:3C:507:3PE:H241	69:3C:508:3PE:C24	2.28	0.58
48:3D:326:TYR:CZ	48:3D:328:PRO:HB3	2.38	0.58
49:3E:190:VAL:HG22	49:3E:250:ARG:CZ	2.33	0.58
69:3P:505:3PE:H242	69:3P:518:3PE:H331	1.85	0.58
5:1E:106:THR:O	5:1E:110:LEU:HG	2.04	0.58
8:1H:146:LEU:HD11	8:1H:192:GLU:HG3	1.86	0.58
12:1L:102:GLU:OE1	12:1L:456:ARG:NH2	2.37	0.58
69:1L:702:3PE:H391	69:1L:702:3PE:H3D2	1.85	0.58
15:1O:75:GLY:HA2	15:1O:99:TRP:CD2	2.39	0.58
24:1Y:13:GLU:HG3	24:1Y:20:LYS:HE3	1.85	0.58
24:1Y:75:ILE:CG2	69:1Y:201:3PE:C28	2.82	0.58
24:1Y:109:ILE:HG12	70:1Y:206:PC1:C32	2.33	0.58
40:1o:77:LEU:CD1	69:1o:201:3PE:H261	2.34	0.58
46:3B:161:GLU:OE1	49:3I:64:LEU:HD11	2.04	0.58
47:3C:104:TYR:HA	47:3C:314:SER:HB2	1.86	0.58
69:3E:303:3PE:H3E2	69:3E:303:3PE:H2B1	1.85	0.58
52:3H:63:GLU:O	52:3H:67:GLN:HG3	2.04	0.58
7:1G:19:MET:HA	7:1G:19:MET:HE3	1.86	0.58
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	1.85	0.58
12:1L:570:GLN:HG3	69:1L:705:3PE:H261	1.86	0.58
16:1P:319:ARG:HA	16:1P:322:ARG:HG3	1.86	0.58
38:1m:87:LEU:HD12	69:1m:202:3PE:C26	2.34	0.58
69:1m:203:3PE:H3A1	69:1m:205:3PE:H3I1	1.85	0.58
75:3N:502:CDL:H651	69:3R:304:3PE:H3G1	1.86	0.58
53:3W:54:LYS:CA	53:3W:57:LYS:HD2	2.31	0.58
55:4A:31:THR:HG21	55:4A:465:VAL:HG11	1.86	0.58
1:1A:23:TRP:O	70:1A:202:PC1:C14	2.52	0.57
69:1A:203:3PE:H291	69:1A:203:3PE:H2D2	1.86	0.57
2:1B:54:CYS:HB3	4:1D:108:TYR:HB3	1.85	0.57
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.85	0.57
6:1F:203:PRO:C	6:1F:404:ILE:HD11	2.28	0.57
7:1G:263:ILE:HA	7:1G:390:LEU:HD11	1.85	0.57
10:1J:52:LEU:O	10:1J:56:VAL:HG23	2.03	0.57
14:1N:326:LEU:O	14:1N:330:ILE:HG12	2.03	0.57
24:1Y:103:ARG:HH12	75:1Y:217:CDL:HB31	1.69	0.57
69:1Y:214:3PE:H241	69:1Y:214:3PE:C35	2.26	0.57
75:1Y:217:CDL:CA5	75:1Y:217:CDL:H141	2.34	0.57
69:1d:203:3PE:H372	75:1d:205:CDL:H791	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1d:206:3PE:C38	69:1f:104:3PE:C29	2.82	0.57
34:1i:88:HIS:HE2	75:1i:201:CDL:PB2	2.26	0.57
75:3A:501:CDL:H131	69:3A:502:3PE:O22	2.04	0.57
49:3R:187:GLU:CD	49:3R:244:ASP:HB2	2.29	0.57
70:1B:203:PC1:H3E1	8:1H:53:LEU:HD11	1.86	0.57
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.86	0.57
14:1N:1:FME:O1	15:1O:258:ARG:NH2	2.36	0.57
69:1Y:215:3PE:H2A2	69:1Y:216:3PE:C2E	2.34	0.57
33:1h:77:ARG:NH1	70:1h:202:PC1:H132	2.19	0.57
40:1o:95:VAL:HA	40:1o:98:MET:HB2	1.87	0.57
47:3C:331:ASP:O	47:3C:334:THR:HG22	2.03	0.57
69:3C:509:3PE:H282	69:3X:107:3PE:H3D1	1.86	0.57
49:3E:265:PHE:HE2	49:3E:269:ASP:HA	1.68	0.57
50:3F:31:TRP:CD1	75:3F:201:CDL:H722	2.39	0.57
45:3N:268:VAL:HB	45:3N:269:PRO:HD3	1.86	0.57
69:3P:507:3PE:H321	69:3P:507:3PE:C22	2.34	0.57
48:3Q:40:CYS:SG	86:3Q:501:HEC:C3C	2.90	0.57
69:3S:201:3PE:H372	70:3T:102:PC1:H261	1.86	0.57
53:3W:30:LEU:HA	54:3X:34:TRP:CD1	2.39	0.57
75:4C:306:CDL:H852	75:4C:306:CDL:H641	1.85	0.57
2:1B:28:TYR:O	2:1B:32:LYS:HG2	2.04	0.57
7:1G:396:ARG:NH1	7:1G:416:THR:O	2.36	0.57
75:1L:704:CDL:H112	13:1M:357:THR:HG21	1.85	0.57
69:1N:401:3PE:C2E	69:1d:201:3PE:H212	2.34	0.57
31:1f:24:CYS:O	31:1f:28:ARG:HD3	2.04	0.57
47:3C:221:HIS:O	47:3C:222:PRO:C	2.47	0.57
69:3N:501:3PE:H3F2	75:3N:502:CDL:H372	1.85	0.57
69:3P:507:3PE:H221	54:3Y:38:TRP:CE2	2.39	0.57
69:3P:508:3PE:H2H2	69:3P:519:3PE:H3G2	1.86	0.57
48:3Q:156:GLN:CG	52:3U:59:PHE:HZ	2.17	0.57
49:3R:173:PRO:O	49:3R:215:GLY:N	2.32	0.57
75:3T:101:CDL:H711	75:3T:101:CDL:C53	2.31	0.57
2:1B:177:TYR:CG	70:1B:202:PC1:H272	2.36	0.57
8:1H:179:TRP:O	8:1H:183:MET:HG3	2.03	0.57
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.33	0.57
12:1L:361:GLY:HA2	36:1k:59:ASN:HD21	1.68	0.57
13:1M:11:LEU:HB3	13:1M:100:ILE:HD13	1.86	0.57
15:1O:95:ARG:HB2	15:1O:281:GLU:O	2.04	0.57
25:1Z:105:LYS:HB3	25:1Z:108:GLU:HB2	1.86	0.57
26:1a:39:ALA:HA	26:1a:44:GLN:HB2	1.85	0.57
29:1d:13:PHE:CD2	69:1d:203:3PE:H231	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:56:TRP:CH2	69:1g:202:3PE:H342	2.38	0.57
69:3E:302:3PE:H332	69:3E:302:3PE:C1	2.30	0.57
46:3O:342:ASP:HA	46:3O:345:LYS:HD3	1.85	0.57
47:3P:132:VAL:HA	47:3P:139:SER:HB3	1.86	0.57
69:3S:201:3PE:H341	69:3S:201:3PE:C28	2.34	0.57
59:4E:84:TYR:O	59:4E:88:GLU:HG2	2.04	0.57
2:1B:176:TRP:CH2	70:1B:202:PC1:C29	2.87	0.57
2:1B:179:ARG:O	16:1P:103:ASN:ND2	2.37	0.57
12:1L:142:ILE:HG22	75:1L:704:CDL:H791	1.85	0.57
70:1Y:207:PC1:H3G2	69:1Y:212:3PE:H2A1	1.86	0.57
47:3C:372:ILE:HG12	69:3C:508:3PE:H252	1.86	0.57
49:3E:141:SER:O	49:3E:142:ALA:C	2.47	0.57
49:3E:219:HIS:C	49:3E:221:GLY:H	2.12	0.57
45:3N:4:TYR:CZ	45:3N:8:LEU:HD11	2.39	0.57
45:3N:237:THR:CG2	51:3T:18:LEU:HD11	2.34	0.57
47:3P:246:SER:HB3	69:3Q:504:3PE:H341	1.85	0.57
47:3P:265:PRO:HD2	47:3P:268:ILE:HD11	1.86	0.57
49:3R:178:HIS:HE1	49:3R:209:GLU:HB3	1.68	0.57
55:4A:117:MET:O	66:4L:46:LYS:NZ	2.37	0.57
1:1A:23:TRP:CE3	70:1P:502:PC1:H242	2.37	0.57
3:1C:151:ILE:HG23	3:1C:152:LEU:HG	1.85	0.57
4:1D:342:MET:HE3	7:1G:103:LEU:HA	1.85	0.57
6:1F:28:ARG:NH1	44:1s:35:ASN:O	2.38	0.57
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.86	0.57
13:1M:84:LEU:HD22	13:1M:87:GLU:HG3	1.86	0.57
15:1O:83:TYR:CB	15:1O:190:HIS:HB3	2.33	0.57
29:1d:113:LEU:HD22	32:1g:121:PRO:HG3	1.87	0.57
47:3C:284:ILE:HD13	69:3C:512:3PE:H352	1.75	0.57
47:3C:306:MET:HA	69:3C:506:3PE:C12	2.34	0.57
48:3D:232:ARG:HD3	49:3R:237:PRO:CB	2.25	0.57
49:3E:181:LYS:HA	49:3E:184:ILE:HG22	1.86	0.57
54:3Y:2:LEU:O	54:3Y:6:LEU:HG	2.04	0.57
55:4A:3:VAL:HG12	55:4A:7:LEU:HD12	1.86	0.57
55:4A:264:LYS:NZ	55:4A:326:THR:O	2.31	0.57
55:4A:423:MET:HB2	91:4A:608:PGV:H181	1.86	0.57
1:1A:92:LEU:HD22	8:1H:302:MET:HG2	1.85	0.57
5:1E:87:TYR:CG	6:1F:181:ALA:HB3	2.40	0.57
5:1E:109:MET:O	5:1E:112:ASN:N	2.36	0.57
69:1L:712:3PE:H3E2	69:1L:204:3PE:H3E2	1.86	0.57
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.36	0.57
24:1Y:22:TYR:CE1	75:1Y:217:CDL:C47	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:114:LEU:HD23	38:1m:119:LYS:HD2	1.87	0.57
69:3C:507:3PE:H2D1	69:3C:508:3PE:H3I3	1.87	0.57
49:3E:169:TRP:HD1	49:3E:214:ILE:HD11	1.68	0.57
49:3E:172:LYS:HB3	49:3E:214:ILE:HG23	1.87	0.57
49:3E:214:ILE:H	49:3E:261:PRO:HD3	1.69	0.57
49:3I:77:ARG:HB3	49:3I:77:ARG:NH1	2.19	0.57
45:3N:358:LYS:HD2	45:3N:402:VAL:HG13	1.87	0.57
47:3P:141:TRP:CD1	47:3P:265:PRO:HD3	2.39	0.57
49:3R:191:GLU:HG3	49:3R:194:GLN:H	1.69	0.57
54:3X:44:TRP:CE2	69:3X:108:3PE:H372	2.40	0.57
58:4D:60:TYR:OH	59:4E:69:GLU:OE1	2.18	0.57
4:1D:261:ARG:NH2	4:1D:368:GLU:OE2	2.38	0.57
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	1.85	0.57
12:1L:105:MET:HB2	12:1L:449:LEU:HD13	1.86	0.57
12:1L:209:PRO:HB2	12:1L:213:LEU:HG	1.87	0.57
69:1L:708:3PE:H31	69:1L:708:3PE:C23	2.35	0.57
13:1M:127:VAL:O	13:1M:131:ILE:HG12	2.04	0.57
13:1M:253:LEU:HD11	13:1M:256:TYR:OH	2.03	0.57
14:1N:133:TRP:HE3	75:1N:402:CDL:C59	2.18	0.57
49:3E:169:TRP:HB2	49:3E:174:LEU:HD22	1.86	0.57
69:3G:103:3PE:H372	69:3G:104:3PE:H371	1.86	0.57
69:3N:503:3PE:H3G2	69:3R:304:3PE:H3I3	1.86	0.57
49:3R:253:PRO:O	49:3R:254:ALA:C	2.48	0.57
55:4A:289:ALA:HB3	55:4A:305:PHE:CD2	2.40	0.57
70:1H:402:PC1:H2B1	9:1I:34:LEU:CD2	2.31	0.57
69:1J:201:3PE:H2I2	69:1J:201:3PE:H3C2	1.87	0.57
69:1L:712:3PE:H242	69:1I:204:3PE:H252	1.86	0.57
24:1Y:108:GLY:C	70:1Y:206:PC1:H232	2.29	0.57
45:3A:170:PRO:HB2	45:3A:172:GLU:CD	2.30	0.57
45:3N:41:ILE:HG12	45:3N:195:MET:HG2	1.86	0.57
49:3R:154:ILE:HD11	49:3R:270:LEU:HA	1.87	0.57
69:3R:302:3PE:H362	69:3R:302:3PE:H3B1	1.86	0.57
52:3U:34:ARG:CZ	52:3U:37:LEU:HD23	2.34	0.57
56:4B:57:ASP:N	93:4B:303:PSC:O13	2.35	0.57
10:1J:115:ILE:O	10:1J:117:PHE:N	2.36	0.57
13:1M:373:ILE:HA	13:1M:376:ILE:HD12	1.87	0.57
18:1R:20:ASP:N	18:1R:20:ASP:OD1	2.38	0.57
24:1Y:8:TYR:CE2	69:1Y:208:3PE:H3H2	2.40	0.57
69:3C:515:3PE:H2	69:3C:515:3PE:H241	1.86	0.57
75:3F:201:CDL:H272	69:3G:109:3PE:H3D2	1.87	0.57
45:3N:49:ASN:N	45:3N:52:ASN:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3P:306:MET:HG2	69:3P:514:3PE:C22	2.34	0.57
49:3R:150:SER:HB3	49:3R:170:ARG:H	1.70	0.57
49:3R:150:SER:HB3	49:3R:170:ARG:N	2.20	0.57
69:3S:201:3PE:H2C1	69:3S:201:3PE:H281	1.86	0.57
54:3X:5:PHE:HZ	69:3X:105:3PE:O12	1.88	0.57
54:3X:39:ARG:HG2	54:3X:52:PHE:CE2	2.40	0.57
54:3X:44:TRP:CH2	69:3X:108:3PE:C37	2.68	0.57
57:4C:86:PHE:CZ	91:4C:305:PGV:H301	2.40	0.57
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.87	0.56
10:1J:41:CYS:HG	10:1J:57:PHE:HD2	1.51	0.56
14:1N:243:LEU:O	14:1N:247:THR:HG23	2.05	0.56
15:1O:133:VAL:CG2	15:1O:202:ILE:HG23	2.31	0.56
16:1P:71:MET:HG3	16:1P:84:VAL:HG12	1.85	0.56
24:1Y:122:ALA:HB1	70:1Y:202:PC1:C35	2.23	0.56
75:1Y:217:CDL:H591	75:1Y:217:CDL:H432	1.87	0.56
45:3A:248:LEU:HD12	45:3A:426:GLY:HA2	1.86	0.56
69:3A:502:3PE:H2F2	69:3E:302:3PE:H2E1	1.87	0.56
46:3B:369:LEU:HD11	46:3B:399:LEU:HD11	1.87	0.56
47:3C:304:MET:HB2	47:3C:305:PRO:HD3	1.86	0.56
69:3C:509:3PE:H321	69:3X:108:3PE:H251	1.86	0.56
49:3E:242:HIS:CB	49:3E:251:LYS:HB3	2.32	0.56
69:3N:501:3PE:H291	75:3X:103:CDL:H671	1.87	0.56
46:3O:411:ILE:O	46:3O:414:ALA:HB3	2.05	0.56
69:3S:201:3PE:C3F	70:3T:102:PC1:H272	2.35	0.56
69:3S:201:3PE:H3F1	70:3T:102:PC1:H272	1.86	0.56
1:1A:18:VAL:O	1:1A:22:PHE:N	2.31	0.56
1:1A:68:GLU:HB3	10:1J:161:LEU:HD13	1.88	0.56
7:1G:226:GLU:OE1	17:1Q:36:ARG:NH2	2.38	0.56
22:1W:31:ARG:NH2	22:1W:80:ASP:OD1	2.37	0.56
69:1Y:214:3PE:C3H	75:3P:513:CDL:H142	2.23	0.56
26:1a:1:MET:CE	75:1q:201:CDL:HB21	2.35	0.56
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.86	0.56
49:3E:80:HIS:HA	49:3E:83:ILE:HD12	1.87	0.56
52:3H:53:GLU:O	52:3H:57:LYS:HG2	2.05	0.56
46:3O:303:VAL:HG21	46:3O:336:VAL:CG2	2.34	0.56
47:3P:253:PRO:O	48:3Q:119:ALA:HA	2.05	0.56
47:3P:320:LEU:CD2	70:3T:102:PC1:H242	2.35	0.56
49:3R:248:ARG:HD2	49:3R:257:ASN:HB3	1.87	0.56
56:4B:160:LEU:HB3	56:4B:198:GLU:HG2	1.87	0.56
5:1E:203:THR:O	44:1s:35:ASN:ND2	2.38	0.56
8:1H:277:TYR:CE2	70:1H:402:PC1:H272	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:59:MET:HE2	14:1N:84:TRP:HH2	1.70	0.56
12:1L:161:ARG:NH1	12:1L:238:GLU:OE2	2.38	0.56
75:1L:704:CDL:H591	13:1M:371:PRO:HD2	1.85	0.56
14:1N:203:LEU:CD1	70:1d:204:PC1:H3D1	2.35	0.56
14:1N:325:LEU:HA	75:1d:205:CDL:OA4	2.05	0.56
22:1W:91:GLU:O	22:1W:95:ASN:ND2	2.32	0.56
23:1X:122:GLY:HA3	27:1b:77:LEU:HG	1.86	0.56
24:1Y:48:PHE:CD1	69:1Y:210:3PE:H231	2.40	0.56
24:1Y:111:ALA:CB	69:1Y:213:3PE:H331	2.35	0.56
24:1Y:112:ALA:HA	70:1Y:206:PC1:C29	2.35	0.56
69:1Y:216:3PE:H2I3	75:1Y:217:CDL:H362	1.87	0.56
38:1m:87:LEU:HB3	69:1m:202:3PE:C25	2.33	0.56
38:1m:87:LEU:CG	69:1m:202:3PE:H251	2.36	0.56
69:1m:202:3PE:H2D2	69:1m:202:3PE:H3B2	1.86	0.56
42:1q:2:GLU:O	42:1q:6:VAL:HG23	2.06	0.56
75:1q:202:CDL:H541	75:1q:202:CDL:H721	1.88	0.56
45:3A:192:ALA:N	45:3A:193:PRO:HD2	2.20	0.56
46:3B:109:VAL:HG13	46:3B:123:LEU:HD13	1.85	0.56
46:3B:435:PHE:HB2	46:3B:438:GLU:HG3	1.87	0.56
47:3C:286:ASN:ND2	69:3C:513:3PE:H12	2.17	0.56
47:3C:337:TRP:CH2	51:3G:61:TYR:HA	2.39	0.56
69:3C:517:3PE:H321	69:4G:101:3PE:C25	2.34	0.56
48:3D:141:GLY:HA2	53:3J:53:TRP:CD1	2.41	0.56
48:3D:215:VAL:O	48:3D:219:LEU:HG	2.05	0.56
48:3D:235:LEU:HD11	49:3R:238:CYS:HA	1.87	0.56
49:3E:266:THR:HB	49:3E:270:LEU:CG	2.35	0.56
69:3N:503:3PE:H3E1	69:3R:304:3PE:H2F2	1.88	0.56
47:3P:286:ASN:ND2	69:3P:503:3PE:H242	2.21	0.56
47:3P:365:LEU:CD2	70:3T:102:PC1:H2I1	2.35	0.56
47:3P:371:ILE:CD1	69:3P:506:3PE:H252	2.35	0.56
48:3Q:16:GLY:HA3	69:3Q:502:3PE:H122	1.88	0.56
49:3R:167:PHE:HB3	49:3R:169:TRP:CZ2	2.41	0.56
69:3W:102:3PE:C36	69:3X:101:3PE:H372	2.35	0.56
69:3W:103:3PE:H2	69:3W:103:3PE:C12	2.33	0.56
69:3X:107:3PE:H2A1	69:4G:101:3PE:H282	1.87	0.56
75:3Y:106:CDL:OA4	75:3Y:106:CDL:H321	2.06	0.56
56:4B:155:SER:HB2	56:4B:179:LEU:HD12	1.86	0.56
75:4B:302:CDL:H181	75:4B:302:CDL:H462	1.87	0.56
68:4N:48:LYS:HD2	68:4N:48:LYS:N	2.20	0.56
2:1B:176:TRP:NE1	70:1B:202:PC1:H222	2.19	0.56
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:96:ILE:HG23	25:1Z:144:THR:CB	2.34	0.56
69:1M:502:3PE:H2G1	69:1L:204:3PE:H3G2	1.86	0.56
24:1Y:2:LYS:O	24:1Y:6:HIS:N	2.37	0.56
24:1Y:62:SER:HG	69:1Y:208:3PE:H341	1.63	0.56
69:1Y:201:3PE:H331	51:3T:56:TYR:CD1	2.38	0.56
69:1Y:205:3PE:O12	69:1Y:208:3PE:H31	2.06	0.56
45:3A:41:ILE:HG12	45:3A:195:MET:HG2	1.87	0.56
46:3B:120:MET:O	46:3B:124:LEU:HD23	2.04	0.56
47:3C:221:HIS:HA	47:3C:225:THR:CG2	2.35	0.56
69:3C:509:3PE:H32	69:3X:108:3PE:O12	2.05	0.56
49:3E:234:TYR:HB2	49:3E:243:TYR:HB3	1.86	0.56
51:3G:63:TRP:CZ2	69:3G:110:3PE:H12	2.41	0.56
69:3G:102:3PE:H251	69:3G:102:3PE:H362	1.87	0.56
69:3J:103:3PE:H2G1	69:3J:103:3PE:C2C	2.22	0.56
46:3O:109:VAL:HG13	46:3O:123:LEU:HD13	1.87	0.56
49:3R:200:HIS:O	49:3R:204:ARG:HG3	2.04	0.56
52:3U:57:GLU:OE1	52:3U:57:GLU:N	2.38	0.56
69:3X:108:3PE:H241	69:3X:108:3PE:H331	1.87	0.56
55:4A:354:THR:HG22	55:4A:376:HIS:HB2	1.87	0.56
56:4B:122:MET:HE1	56:4B:206:PHE:HD2	1.71	0.56
57:4C:83:MET:HG3	57:4C:237:ALA:HB1	1.87	0.56
59:4E:44:GLU:HG2	59:4E:45:PRO:HD2	1.87	0.56
1:1A:23:TRP:HE1	70:1A:202:PC1:C21	2.19	0.56
3:1C:116:PRO:HD2	22:1W:18:LYS:HE2	1.86	0.56
4:1D:78:PRO:HG3	4:1D:402:LEU:HD23	1.86	0.56
9:1I:45:PRO:O	76:1I:203:AYA:HM1	2.05	0.56
12:1L:562:LEU:HB2	12:1L:563:PRO:CD	2.35	0.56
13:1M:69:THR:HG22	13:1M:234:VAL:HG11	1.88	0.56
13:1M:127:VAL:HG11	69:1N:401:3PE:H3F2	1.86	0.56
14:1N:218:LEU:HB3	14:1N:244:MET:HE2	1.87	0.56
70:1P:502:PC1:H241	70:1P:502:PC1:H111	1.85	0.56
19:1S:64:LEU:HB3	19:1S:76:VAL:HG13	1.87	0.56
31:1f:21:VAL:CG2	69:1f:104:3PE:H3E2	2.30	0.56
46:3B:276:GLN:HG2	46:3B:281:ALA:HB2	1.86	0.56
49:3E:121:THR:O	49:3E:125:VAL:HG23	2.05	0.56
49:3E:249:ILE:N	49:3E:257:ASN:HB3	2.20	0.56
69:3P:503:3PE:H282	69:3P:518:3PE:H332	1.88	0.56
69:3P:507:3PE:H231	69:3P:507:3PE:H341	1.88	0.56
69:3P:508:3PE:C2H	69:3P:519:3PE:H3G2	2.36	0.56
55:4A:230:LEU:HB2	57:4C:103:HIS:CD2	2.41	0.56
12:1L:146:GLY:CA	75:1L:704:CDL:H762	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1Y:205:3PE:H292	70:1Y:206:PC1:C3E	2.36	0.56
26:1a:1:MET:HE1	75:1q:201:CDL:HB21	1.86	0.56
39:1n:55:ASP:HB2	45:3N:193:PRO:HG2	1.87	0.56
45:3A:287:GLY:N	45:3A:290:MET:HE3	2.20	0.56
46:3B:95:LYS:CE	49:3I:72:VAL:HB	2.36	0.56
46:3B:200:THR:HB	46:3B:227:ARG:CG	2.28	0.56
69:3Q:503:3PE:H2F2	69:3W:101:3PE:C3C	2.35	0.56
49:3R:131:ASN:HB3	69:3R:302:3PE:H222	1.88	0.56
2:1B:41:ARG:NH2	8:1H:57:THR:HG22	2.21	0.56
5:1E:16:ASN:ND2	5:1E:19:THR:OG1	2.39	0.56
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.39	0.56
12:1L:206:ASN:OD1	12:1L:206:ASN:N	2.38	0.56
15:1O:97:GLN:HE21	15:1O:135:LEU:HB2	1.71	0.56
24:1Y:28:GLY:CA	69:1Y:208:3PE:H382	2.36	0.56
69:1d:201:3PE:H2H1	75:1d:202:CDL:H461	1.88	0.56
38:1m:99:PHE:CD2	69:1m:205:3PE:C3H	2.89	0.56
45:3A:444:LEU:HB2	75:3A:501:CDL:HB61	1.88	0.56
47:3C:281:LEU:HD13	47:3C:294:LEU:HD13	1.86	0.56
69:3C:516:3PE:C22	69:3Y:107:3PE:H322	2.34	0.56
49:3R:219:HIS:HB2	72:3R:301:FES:S2	2.46	0.56
49:3R:231:PHE:CD1	49:3R:250:ARG:HG3	2.41	0.56
69:3S:201:3PE:H232	69:3S:201:3PE:C3	2.23	0.56
51:3T:29:TYR:H	69:3T:103:3PE:H2I3	1.70	0.56
70:3X:104:PC1:H272	70:3X:104:PC1:H321	1.87	0.56
61:4G:70:PHE:O	87:4G:103:PEK:N	2.39	0.56
4:1D:65:VAL:HB	4:1D:77:ASP:HB3	1.86	0.56
6:1F:95:VAL:HB	6:1F:136:ILE:HG13	1.87	0.56
12:1L:188:TRP:HZ3	12:1L:206:ASN:HD22	1.51	0.56
69:1L:705:3PE:H3F2	82:1Y:203:PGT:C45	2.36	0.56
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.39	0.56
69:1N:401:3PE:H12	69:1N:401:3PE:HN1	1.71	0.56
15:1O:260:ARG:HA	15:1O:263:VAL:HB	1.88	0.56
28:1c:43:LYS:HG2	28:1c:48:LEU:HD23	1.88	0.56
69:3C:508:3PE:H3G1	69:3G:109:3PE:H3A2	1.88	0.56
69:3J:102:3PE:O12	69:3J:102:3PE:N	2.38	0.56
69:3N:501:3PE:H332	47:3P:5:ARG:HB2	1.87	0.56
75:3N:502:CDL:H521	75:3N:502:CDL:HB62	1.88	0.56
46:3O:214:PRO:O	46:3O:218:GLN:HG2	2.06	0.56
54:3X:44:TRP:HZ2	69:3X:108:3PE:C21	2.18	0.56
70:1B:203:PC1:H232	69:1B:204:3PE:O32	2.06	0.56
7:1G:135:ARG:HH21	7:1G:155:GLN:HE22	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:220:HIS:O	13:1M:228:SER:OG	2.23	0.56
15:1O:38:LEU:HD11	15:1O:234:VAL:HG21	1.87	0.56
15:1O:125:GLU:O	15:1O:126:ARG:HB2	2.06	0.56
24:1Y:43:LYS:O	24:1Y:54:ARG:NH1	2.36	0.56
24:1Y:109:ILE:HG23	70:1Y:206:PC1:C34	2.36	0.56
69:1Y:214:3PE:H2G2	69:1Y:216:3PE:H2I1	1.87	0.56
37:1I:124:SER:O	37:1I:124:SER:OG	2.23	0.56
47:3C:289:GLY:HA3	69:3C:512:3PE:C33	2.36	0.56
48:3D:93:LEU:HD23	48:3D:239:PRO:HB2	1.88	0.56
48:3D:307:LEU:HB3	49:3E:121:THR:OG1	2.06	0.56
69:3D:502:3PE:H12	69:3J:101:3PE:H222	1.87	0.56
46:3O:70:ARG:O	49:3V:68:VAL:HG21	2.05	0.56
69:3P:508:3PE:H3C2	69:3P:508:3PE:H382	1.88	0.56
70:3P:509:PC1:H3F2	69:3P:514:3PE:H3I1	1.88	0.56
75:3Y:106:CDL:OA6	75:3Y:106:CDL:HA21	2.06	0.56
7:1G:199:ILE:HG23	7:1G:208:LEU:HD13	1.88	0.56
7:1G:241:SER:HB2	7:1G:249:ARG:HG3	1.88	0.56
10:1J:91:GLY:HA3	69:1J:201:3PE:H331	1.86	0.56
13:1M:128:PRO:O	13:1M:132:ILE:HG12	2.05	0.56
23:1X:171:MET:HE1	29:1d:29:PRO:HD2	1.87	0.56
24:1Y:120:THR:HG23	69:1Y:211:3PE:H2F2	1.88	0.56
38:1m:92:PHE:CE1	69:1m:203:3PE:C27	2.85	0.56
69:1m:201:3PE:H12	69:1m:201:3PE:C12	2.36	0.56
75:3A:501:CDL:H641	69:3A:502:3PE:H2H1	1.88	0.56
69:3C:507:3PE:H291	69:3C:508:3PE:H281	1.88	0.56
69:3P:514:3PE:H2F1	69:3P:518:3PE:H3I3	1.87	0.56
50:3S:59:VAL:HG11	51:3T:10:MET:HG2	1.88	0.56
3:1C:68:THR:N	21:1V:86:GLU:OE1	2.39	0.55
6:1F:197:GLU:OE2	17:1Q:129:ARG:NH1	2.35	0.55
12:1L:6:SER:O	12:1L:10:THR:OG1	2.23	0.55
15:1O:136:GLU:O	15:1O:139:TYR:HB3	2.05	0.55
20:1T:47:GLN:HE22	20:1T:68:GLU:HA	1.72	0.55
20:1U:4:PRO:HG3	35:1j:9:PRO:HG2	1.87	0.55
75:1Y:217:CDL:HB21	50:3S:19:TRP:CD1	2.40	0.55
69:3C:509:3PE:H351	69:4G:104:3PE:H2B1	1.88	0.55
48:3D:227:THR:HG22	52:3H:69:VAL:HB	1.88	0.55
51:3G:56:VAL:HG21	69:3G:109:3PE:C2A	2.14	0.55
45:3N:49:ASN:O	45:3N:53:ASN:HB2	2.06	0.55
69:3N:501:3PE:H112	69:3P:511:3PE:C12	2.35	0.55
46:3O:209:LEU:HD21	46:3O:378:PHE:HD2	1.70	0.55
48:3Q:16:GLY:CA	69:3Q:502:3PE:H122	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3Q:237:TYR:CZ	48:3Q:239:PRO:HB3	2.41	0.55
49:3R:172:LYS:HB3	49:3R:214:ILE:HG23	1.88	0.55
49:3R:184:ILE:HG21	49:3R:208:PRO:HB3	1.86	0.55
75:3T:101:CDL:H531	75:3T:101:CDL:C71	2.33	0.55
62:4H:56:TYR:CZ	68:4N:80:PRO:HD2	2.40	0.55
4:1D:166:PRO:HG3	4:1D:228:MET:HG3	1.88	0.55
6:1F:362:CYS:HG	71:1F:502:SF4:FE4	1.22	0.55
7:1G:551:ASP:OD2	7:1G:679:ARG:NE	2.39	0.55
10:1J:21:SER:HA	11:1K:32:CYS:SG	2.46	0.55
13:1M:7:PRO:HG3	31:1f:20:PHE:HA	1.88	0.55
14:1N:309:ASN:ND2	15:1O:95:ARG:HG3	2.21	0.55
15:1O:81:LYS:O	15:1O:81:LYS:HG2	2.06	0.55
32:1g:52:ILE:HG13	69:1g:202:3PE:H2	1.88	0.55
75:1g:201:CDL:H772	33:1h:34:ILE:HG21	1.87	0.55
40:1o:75:ASN:HD21	69:1o:201:3PE:H221	1.70	0.55
69:3E:302:3PE:H291	69:3E:302:3PE:H3I3	1.89	0.55
51:3G:44:ARG:HG3	69:3G:106:3PE:O12	2.06	0.55
69:3G:106:3PE:H322	69:3G:106:3PE:C22	2.36	0.55
55:4A:101:SER:OG	55:4A:156:SER:O	2.25	0.55
57:4C:88:ILE:HG12	75:4C:306:CDL:H631	1.88	0.55
91:4C:302:PGV:H012	91:4C:302:PGV:C6	2.36	0.55
7:1G:199:ILE:HG12	7:1G:202:ILE:HD11	1.89	0.55
7:1G:364:LEU:HD12	7:1G:491:ASN:HB3	1.88	0.55
75:1L:704:CDL:H331	75:1L:704:CDL:OB7	2.06	0.55
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.41	0.55
14:1N:73:ALA:HB2	14:1N:97:MET:HB3	1.87	0.55
75:1g:201:CDL:OB9	33:1h:30:LEU:HB3	2.06	0.55
69:3A:502:3PE:H2F2	69:3E:302:3PE:C2E	2.37	0.55
47:3C:359:PHE:HB3	69:3C:512:3PE:H2H2	1.87	0.55
69:3C:515:3PE:H2H2	69:3C:516:3PE:H2C1	1.89	0.55
69:3D:503:3PE:H3H2	69:3D:503:3PE:H3B1	1.88	0.55
69:3E:302:3PE:H2	69:3E:302:3PE:H341	1.88	0.55
69:3E:302:3PE:H282	54:3Y:35:ALA:HB1	1.88	0.55
49:3I:42:VAL:HG13	49:3I:43:LEU:HD13	1.88	0.55
69:3P:504:3PE:H342	69:3P:504:3PE:H252	1.88	0.55
48:3Q:27:ARG:HB2	48:3Q:55:CYS:HB2	1.88	0.55
49:3R:218:THR:HB	49:3R:254:ALA:HB1	1.87	0.55
69:3R:302:3PE:H3B2	70:3R:303:PC1:H3B2	1.88	0.55
54:3X:18:ILE:CG1	75:3X:103:CDL:H212	2.36	0.55
5:1E:51:LEU:HD23	5:1E:69:VAL:HG21	1.88	0.55
8:1H:111:LEU:HD11	10:1J:57:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:277:TYR:HE2	70:1H:402:PC1:H292	1.69	0.55
12:1L:2:ASN:HB2	12:1L:3:PRO:HD2	1.87	0.55
12:1L:504:LEU:HD21	64:4J:30:ILE:CD1	2.36	0.55
69:1L:711:3PE:H2	69:1M:502:3PE:H111	1.88	0.55
24:1Y:113:ALA:CA	70:1Y:206:PC1:H372	2.37	0.55
25:1Z:138:TYR:CD2	25:1Z:142:TRP:CZ2	2.94	0.55
25:1Z:138:TYR:HB3	25:1Z:142:TRP:CE2	2.41	0.55
75:1g:201:CDL:H341	69:1g:203:3PE:H262	1.88	0.55
46:3B:207:ILE:HD13	46:3B:383:GLY:HA2	1.87	0.55
49:3I:36:ALA:C	49:3I:38:SER:H	2.13	0.55
53:3J:53:TRP:CH2	53:3J:60:TYR:HD2	2.24	0.55
47:3P:92:ILE:O	47:3P:96:ILE:HG13	2.07	0.55
47:3P:157:GLY:O	47:3P:161:VAL:HG23	2.07	0.55
54:3X:5:PHE:CE2	69:3X:105:3PE:C22	2.88	0.55
56:4B:43:SER:O	56:4B:47:THR:OG1	2.18	0.55
6:1F:247:ARG:HB2	6:1F:250:ASN:HD21	1.70	0.55
8:1H:107:ALA:HA	10:1J:58:LEU:HD13	1.89	0.55
69:1L:706:3PE:O12	14:1N:152:ASN:ND2	2.40	0.55
38:1m:39:ARG:NH1	38:1m:39:ARG:HB2	2.21	0.55
47:3P:286:ASN:HD21	69:3P:503:3PE:P	2.29	0.55
52:3U:27:ILE:HG12	52:3U:30:CYS:HB2	1.88	0.55
75:3X:103:CDL:HB62	75:3X:103:CDL:H541	1.89	0.55
54:3Y:19:PRO:HB3	69:3Y:101:3PE:H322	1.87	0.55
55:4A:313:ALA:HB2	55:4A:356:ILE:HD11	1.89	0.55
91:4A:607:PGV:H41	68:4N:1:MET:HE3	1.87	0.55
56:4B:41:ILE:O	56:4B:45:MET:HG2	2.06	0.55
57:4C:157:LYS:HE3	91:4C:302:PGV:H51	1.88	0.55
57:4C:224:LYS:NZ	75:4C:307:CDL:HB4	2.21	0.55
6:1F:19:ASP:HB3	6:1F:245:PHE:HE2	1.71	0.55
8:1H:49:ILE:O	8:1H:53:LEU:HD13	2.06	0.55
8:1H:173:TRP:NE1	70:1H:404:PC1:H122	2.22	0.55
15:1O:202:ILE:O	15:1O:206:TYR:HB2	2.06	0.55
75:1q:202:CDL:H172	75:1q:202:CDL:H602	1.89	0.55
47:3C:326:TRP:NE1	51:3G:50:VAL:HG22	2.21	0.55
47:3P:377:LEU:HG	50:3S:20:TYR:CE2	2.39	0.55
69:3P:506:3PE:H2A2	69:3P:506:3PE:C36	2.36	0.55
69:3Y:102:3PE:O12	69:3Y:102:3PE:H31	2.07	0.55
55:4A:227:ASP:HB2	91:4C:303:PGV:O05	2.05	0.55
91:4G:102:PGV:O04	91:4G:102:PGV:H032	2.06	0.55
7:1G:43:HIS:CE1	7:1G:261:GLU:OE2	2.60	0.55
8:1H:264:LEU:HD13	26:1a:9:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1H:403:PC1:H372	10:1J:57:PHE:HZ	1.71	0.55
69:1L:705:3PE:H3E2	82:1Y:203:PGT:H482	1.87	0.55
20:1T:66:ASP:HA	20:1T:69:LYS:HG3	1.88	0.55
21:1V:36:GLN:HB2	21:1V:94:LEU:HD11	1.89	0.55
70:1Y:207:PC1:H3E2	69:1Y:212:3PE:H2D1	1.88	0.55
25:1Z:34:SER:O	25:1Z:38:VAL:HG23	2.07	0.55
69:1k:101:3PE:H232	69:1o:201:3PE:H231	1.89	0.55
45:3A:260:PRO:HG2	45:3A:267:ASN:OD1	2.06	0.55
46:3B:128:ALA:C	46:3B:130:PRO:HD3	2.31	0.55
47:3C:26:ASN:HD21	47:3C:207:ASN:ND2	2.05	0.55
47:3C:284:ILE:HG21	69:3C:512:3PE:C35	2.36	0.55
46:3O:24:LEU:HD23	46:3O:392:TYR:CG	2.42	0.55
47:3P:146:ILE:HG13	47:3P:147:THR:N	2.22	0.55
47:3P:149:LEU:HA	47:3P:287:LYS:HE3	1.88	0.55
69:3S:201:3PE:H372	70:3T:102:PC1:H231	1.88	0.55
75:3Y:106:CDL:H341	75:3Y:106:CDL:H162	1.87	0.55
57:4C:54:MET:HE1	91:4C:305:PGV:H132	1.87	0.55
65:4K:8:ASP:OD1	65:4K:8:ASP:N	2.40	0.55
5:1E:151:ALA:HB1	5:1E:152:PRO:CD	2.37	0.55
5:1E:184:PRO:HG2	44:1s:44:HIS:CD2	2.42	0.55
6:1F:364:PRO:HB2	6:1F:403:THR:CG2	2.37	0.55
7:1G:453:LEU:HD21	7:1G:458:LEU:HD21	1.89	0.55
10:1J:119:PHE:CE1	11:1K:6:MET:HB2	2.42	0.55
12:1L:473:PRO:HG2	12:1L:475:MET:HE3	1.89	0.55
24:1Y:62:SER:CB	69:1Y:208:3PE:C37	2.42	0.55
69:1d:203:3PE:C2C	75:1d:205:CDL:H622	2.37	0.55
31:1f:22:PHE:CZ	69:1f:104:3PE:H352	2.42	0.55
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.38	0.55
49:3E:132:ALA:HB1	69:3E:303:3PE:H2A2	1.89	0.55
49:3E:237:PRO:O	48:3Q:144:ARG:CG	2.54	0.55
69:3G:108:3PE:H2	69:3G:108:3PE:H231	1.88	0.55
75:3N:502:CDL:H422	47:3P:39:ILE:HD11	1.89	0.55
46:3O:324:ILE:HD11	46:3O:344:VAL:HG21	1.88	0.55
48:3Q:31:GLN:HA	48:3Q:34:LYS:HG2	1.89	0.55
50:3S:51:PRO:HG2	50:3S:54:LEU:HD12	1.87	0.55
1:1A:5:LEU:CD1	8:1H:3:MET:HE1	2.32	0.55
1:1A:27:LEU:HD13	70:1A:202:PC1:H153	1.88	0.55
7:1G:298:ASP:OD1	7:1G:302:ARG:NH2	2.39	0.55
13:1M:127:VAL:HB	69:1N:401:3PE:H3H1	1.87	0.55
70:1M:501:PC1:O13	70:1M:501:PC1:H132	2.06	0.55
69:1Y:215:3PE:H322	69:1Y:216:3PE:H251	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:117:PRO:O	34:1i:117:PRO:HD2	2.06	0.55
48:3D:128:CYS:SG	86:3D:501:HEC:CAC	2.95	0.55
53:3J:53:TRP:CZ3	53:3J:60:TYR:CD2	2.94	0.55
45:3N:244:ARG:HG2	51:3T:10:MET:HB3	1.89	0.55
91:4A:607:PGV:C19	75:4C:306:CDL:HA61	2.36	0.55
69:1A:201:3PE:H392	69:1b:101:3PE:C26	2.36	0.55
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.72	0.55
37:1l:157:GLU:O	40:1o:33:ARG:NH2	2.40	0.55
75:3F:201:CDL:H381	75:3F:201:CDL:H421	1.88	0.55
75:3F:201:CDL:H552	75:3F:201:CDL:H711	1.88	0.55
75:3N:502:CDL:H841	75:3X:103:CDL:H811	1.89	0.55
48:3Q:8:PRO:HG3	52:3U:66:ASP:HB3	1.88	0.55
49:3R:243:TYR:CE1	49:3R:249:ILE:HD13	2.42	0.55
56:4B:120:SER:OG	56:4B:140:ASN:O	2.22	0.55
9:1I:77:CYS:SG	71:1I:202:SF4:FE4	1.86	0.54
9:1I:127:PRO:O	18:1R:69:PRO:HD3	2.07	0.54
12:1L:463:PHE:HB3	69:1L:703:3PE:H242	1.89	0.54
69:1L:709:3PE:C2E	75:1i:201:CDL:H182	2.37	0.54
15:1O:100:LEU:HD21	77:1O:401:GTP:C6	2.42	0.54
69:1Y:201:3PE:H342	69:1Y:201:3PE:H392	1.88	0.54
29:1d:14:LEU:HD23	69:1d:203:3PE:O22	2.07	0.54
34:1i:71:VAL:O	34:1i:76:ILE:HD12	2.07	0.54
38:1m:87:LEU:CB	69:1m:202:3PE:H251	2.36	0.54
46:3B:181:TYR:CZ	46:3B:182:ARG:HG2	2.42	0.54
46:3B:397:THR:O	46:3B:400:GLN:HG2	2.08	0.54
47:3C:95:PHE:CE1	69:3C:503:3PE:H3D1	2.41	0.54
69:3C:507:3PE:H272	69:3C:507:3PE:H341	1.89	0.54
48:3D:106:LEU:HD22	48:3D:295:LEU:HB2	1.89	0.54
50:3F:24:TRP:HE1	50:3F:26:GLU:HB2	1.72	0.54
69:3J:105:3PE:H2A2	54:3Y:46:PRO:HB2	1.88	0.54
47:3P:13:ILE:HG13	47:3P:14:ILE:N	2.21	0.54
49:3R:236:CYS:H	49:3R:242:HIS:HA	1.72	0.54
49:3R:247:GLY:O	49:3R:257:ASN:HB2	2.07	0.54
50:3S:109:LYS:HB3	54:3Y:7:GLY:HA3	1.88	0.54
57:4C:132:LEU:HD21	61:4G:32:THR:HG23	1.89	0.54
1:1A:108:GLN:NE2	69:1A:203:3PE:H242	2.21	0.54
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.40	0.54
24:1Y:111:ALA:HB1	70:1Y:206:PC1:H282	1.89	0.54
29:1d:13:PHE:HE1	70:1d:204:PC1:H352	1.72	0.54
75:1g:201:CDL:H711	33:1h:27:PHE:CE1	2.42	0.54
47:3C:289:GLY:HA3	69:3C:512:3PE:H351	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3C:506:3PE:H252	69:3C:506:3PE:H321	1.89	0.54
48:3D:136:TYR:HA	48:3D:139:LEU:HD12	1.90	0.54
45:3N:174:VAL:HG23	45:3N:175:ARG:HG3	1.89	0.54
69:3P:511:3PE:H382	69:3P:512:3PE:H362	1.89	0.54
49:3R:196:ARG:O	49:3R:198:PRO:HD3	2.08	0.54
49:3R:199:GLN:HB3	49:3R:204:ARG:HD2	1.89	0.54
55:4A:419:VAL:HG22	91:4A:608:PGV:C13	2.33	0.54
69:1B:205:3PE:H371	69:1B:205:3PE:H3B2	1.88	0.54
5:1E:154:VAL:HG22	5:1E:155:GLN:H	1.70	0.54
10:1J:103:MET:HE2	10:1J:115:ILE:HD13	1.90	0.54
13:1M:10:MET:HE1	69:1f:104:3PE:H382	1.89	0.54
31:1f:21:VAL:CG2	69:1f:104:3PE:C3G	2.82	0.54
42:1q:64:TYR:HB2	42:1q:77:VAL:HG11	1.89	0.54
46:3B:249:GLY:O	46:3B:250:ASP:C	2.49	0.54
47:3C:106:SER:HB3	85:3C:502:HEM:HBD2	1.89	0.54
47:3C:109:PHE:HB3	47:3C:112:THR:HG23	1.89	0.54
51:3G:40:LEU:O	51:3G:44:ARG:HG2	2.06	0.54
69:3G:102:3PE:O21	69:3G:102:3PE:H242	2.08	0.54
69:3G:103:3PE:H341	69:3G:103:3PE:H262	1.88	0.54
53:3J:34:ARG:HG2	54:3Y:47:TYR:CE2	2.42	0.54
69:3J:101:3PE:H3C2	69:3J:104:3PE:H371	1.89	0.54
69:3P:518:3PE:H272	69:3P:518:3PE:H322	1.89	0.54
48:3Q:225:HIS:CE1	51:3T:20:PRO:HB2	2.42	0.54
50:3S:12:TRP:CE2	50:3S:14:GLU:HB2	2.43	0.54
69:3X:101:3PE:H291	69:3X:101:3PE:H2D2	1.89	0.54
57:4C:55:TYR:HD1	75:4C:307:CDL:H761	1.72	0.54
58:4D:89:ILE:HG22	65:4K:29:TRP:HE1	1.71	0.54
10:1J:76:THR:OG1	10:1J:77:GLU:N	2.40	0.54
10:1J:175:ASN:O	15:1O:254:ARG:NH2	2.36	0.54
12:1L:78:LEU:HD11	75:1L:704:CDL:C87	2.37	0.54
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.43	0.54
12:1L:288:THR:HG21	12:1L:307:SER:HB3	1.88	0.54
69:3A:502:3PE:H341	69:3A:502:3PE:O31	2.07	0.54
46:3B:299:VAL:CG2	46:3B:309:VAL:HG11	2.34	0.54
69:3C:513:3PE:H381	69:3C:513:3PE:C2B	2.37	0.54
48:3D:329:PRO:HD3	51:3G:14:HIS:CE1	2.42	0.54
49:3E:221:GLY:O	49:3E:222:CYS:C	2.48	0.54
69:3J:105:3PE:H2E1	69:3Y:102:3PE:C38	2.37	0.54
46:3O:86:THR:HG23	49:3V:70:LEU:HD11	1.90	0.54
46:3O:243:GLU:HG3	46:3O:424:MET:HB3	1.88	0.54
48:3Q:180:SER:OG	52:3U:15:ASP:OD1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:222:CYS:O	49:3R:223:VAL:C	2.50	0.54
50:3S:58:ARG:HA	50:3S:61:ARG:NH1	2.23	0.54
53:3W:43:ILE:HG12	69:3W:101:3PE:H342	1.89	0.54
69:3X:108:3PE:H321	69:4G:104:3PE:H31	1.89	0.54
6:1F:363:THR:HG21	7:1G:97:LEU:HG	1.90	0.54
8:1H:24:GLU:OE1	8:1H:274:ARG:NH1	2.40	0.54
8:1H:105:MET:HE3	8:1H:237:PHE:CD2	2.43	0.54
8:1H:197:PRO:HD2	8:1H:198:PHE:CD2	2.42	0.54
14:1N:336:VAL:CG2	69:1d:203:3PE:C2H	2.86	0.54
24:1Y:80:ARG:NE	24:1Y:88:ASN:HD21	2.03	0.54
69:1Y:209:3PE:H381	75:3P:513:CDL:C85	2.37	0.54
37:1l:96:VAL:HG12	37:1l:101:MET:HG3	1.89	0.54
46:3B:153:GLN:OE1	49:3l:46:LYS:HE3	2.07	0.54
47:3C:226:ILE:HD11	48:3D:311:MET:HE2	1.90	0.54
69:3C:516:3PE:H2A2	69:3Y:107:3PE:C3D	2.35	0.54
48:3D:135:ALA:HA	48:3D:178:TYR:HA	1.88	0.54
48:3D:316:TRP:O	48:3D:320:LYS:HG2	2.08	0.54
49:3E:109:ALA:HA	53:3J:7:THR:HG23	1.90	0.54
69:3N:503:3PE:C25	70:3R:303:PC1:H222	2.33	0.54
47:3P:101:GLY:HA2	47:3P:106:SER:HB2	1.90	0.54
69:3P:507:3PE:H2F2	69:3Y:104:3PE:H3C1	1.88	0.54
49:3R:113:PHE:HE1	69:3R:305:3PE:H291	1.72	0.54
52:3U:47:ARG:HB3	52:3U:50:THR:OG1	2.08	0.54
59:4E:16:VAL:HG23	59:4E:47:ILE:HG22	1.90	0.54
2:1B:44:SER:CB	8:1H:54:LYS:HD3	2.33	0.54
70:1B:203:PC1:H332	69:1B:204:3PE:H382	1.89	0.54
69:1J:201:3PE:O14	69:1J:201:3PE:H31	2.08	0.54
12:1L:337:ALA:O	12:1L:341:MET:HG3	2.08	0.54
69:1L:706:3PE:H11	69:1L:706:3PE:O22	2.08	0.54
14:1N:302:LEU:HD23	69:1N:401:3PE:H351	1.89	0.54
15:1O:22:SER:OG	15:1O:119:GLY:O	2.26	0.54
24:1Y:65:ILE:HG22	69:1Y:208:3PE:H3A1	1.88	0.54
24:1Y:95:ALA:HB2	70:1Y:207:PC1:C3C	2.30	0.54
75:1g:201:CDL:H641	75:1g:201:CDL:H382	1.90	0.54
45:3A:211:LEU:HA	45:3A:214:LYS:HG2	1.88	0.54
47:3C:120:LEU:HG	47:3C:124:MET:HE2	1.89	0.54
48:3D:225:PRO:HB2	48:3D:229:VAL:HG22	1.88	0.54
49:3E:192:VAL:O	49:3E:198:PRO:HA	2.07	0.54
49:3R:123:VAL:HG13	53:3W:29:ALA:HA	1.90	0.54
49:3R:179:ARG:NH1	49:3R:211:VAL:HB	2.21	0.54
75:3X:103:CDL:OB7	75:3X:103:CDL:HB32	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:4G:56:ARG:NH1	61:4G:66:ASN:O	2.41	0.54
69:4G:104:3PE:H261	69:4G:104:3PE:H332	1.90	0.54
69:1A:203:3PE:H231	14:1N:4:ILE:HG21	1.90	0.54
2:1B:116:MET:HG3	2:1B:151:PRO:HG2	1.90	0.54
12:1L:23:ASN:HB2	69:1L:709:3PE:O14	2.04	0.54
12:1L:504:LEU:CD1	69:1L:707:3PE:HN3	2.11	0.54
13:1M:307:TRP:HB3	13:1M:384:ALA:HB2	1.90	0.54
31:1f:14:ILE:HG22	69:1f:102:3PE:H2C2	1.90	0.54
39:1n:41:CYS:HA	39:1n:44:ARG:HB3	1.89	0.54
47:3C:172:LYS:O	47:3C:176:THR:HG22	2.07	0.54
47:3C:287:LYS:CG	69:3C:513:3PE:H122	2.37	0.54
49:3E:169:TRP:CE3	49:3E:273:VAL:HA	2.42	0.54
51:3G:63:TRP:CZ2	69:3G:110:3PE:C1	2.91	0.54
53:3J:57:LYS:C	53:3J:58:HIS:CD2	2.84	0.54
46:3O:71:LEU:HD22	46:3O:144:LEU:HD23	1.89	0.54
46:3O:247:GLN:HA	46:3O:428:GLY:O	2.08	0.54
46:3O:291:ALA:HA	46:3O:297:GLN:NE2	2.23	0.54
47:3P:330:ALA:CB	69:3P:510:3PE:H2G2	2.37	0.54
6:1F:100:GLY:HA3	6:1F:184:TYR:HD1	1.71	0.54
8:1H:173:TRP:NE1	70:1H:404:PC1:H111	2.19	0.54
11:1K:5:TYR:HB3	11:1K:43:MET:HE1	1.88	0.54
20:1T:78:ASP:N	20:1T:78:ASP:OD1	2.41	0.54
24:1Y:62:SER:OG	69:1Y:208:3PE:C33	2.56	0.54
47:3C:359:PHE:CD1	69:3C:511:3PE:H3E1	2.43	0.54
69:3C:511:3PE:H31	69:3C:511:3PE:H231	1.90	0.54
51:3G:48:LEU:O	69:3G:109:3PE:H221	2.08	0.54
47:3P:306:MET:HE3	69:3P:514:3PE:H261	1.72	0.54
69:3W:102:3PE:H322	69:3X:101:3PE:C33	2.37	0.54
55:4A:289:ALA:HA	55:4A:292:MET:CE	2.37	0.54
57:4C:251:PHE:CE1	91:4C:303:PGV:H161	2.43	0.54
4:1D:259:MET:HE1	4:1D:421:GLN:HA	1.89	0.54
5:1E:109:MET:O	5:1E:110:LEU:C	2.50	0.54
8:1H:87:VAL:HG22	8:1H:88:PRO:HD3	1.90	0.54
69:1J:201:3PE:H372	69:1J:203:3PE:H261	1.89	0.54
12:1L:24:SER:HB3	69:1L:710:3PE:O21	2.08	0.54
69:1N:401:3PE:H2B1	69:1d:201:3PE:H2G1	1.89	0.54
69:1k:101:3PE:H3C1	69:1k:101:3PE:H3G1	1.89	0.54
81:1n:201:EHZ:O1	81:1n:201:EHZ:S1	2.66	0.54
48:3D:129:HIS:CE1	48:3D:199:PRO:HD2	2.40	0.54
51:3G:75:ASN:C	51:3G:82:PRO:N	2.65	0.54
45:3N:102:LEU:HD21	46:3O:366:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:202:ALA:HB3	46:3O:229:GLY:O	2.08	0.54
46:3O:203:ARG:HD2	46:3O:230:LEU:O	2.07	0.54
47:3P:248:ASP:HB3	69:3P:520:3PE:H121	1.89	0.54
69:3R:305:3PE:H2A1	69:3R:305:3PE:H331	1.90	0.54
55:4A:92:MET:HE3	55:4A:163:ASN:ND2	2.15	0.54
91:4C:302:PGV:H012	91:4C:302:PGV:H41	1.90	0.54
61:4G:62:TRP:HH2	87:4G:103:PEK:H222	1.71	0.54
62:4H:8:ILE:HD11	62:4H:55:TRP:HB2	1.89	0.54
66:4L:15:VAL:HG12	66:4L:21:LEU:HG	1.90	0.54
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.41	0.54
12:1L:272:LEU:HD11	69:1L:712:3PE:H322	1.88	0.54
13:1M:22:MET:CE	69:1g:202:3PE:H221	2.21	0.54
29:1d:120:ARG:HD2	38:1m:115:ILE:HD13	1.90	0.54
69:1f:103:3PE:H291	69:1f:103:3PE:H372	1.90	0.54
69:1m:204:3PE:H3G2	69:1m:204:3PE:H2C2	1.89	0.54
40:1o:77:LEU:HB2	69:1o:201:3PE:C26	2.19	0.54
69:3C:507:3PE:H2G1	69:3C:507:3PE:H3A1	1.89	0.54
50:3F:110:ILE:O	50:3F:114:LYS:HG2	2.08	0.54
49:3R:242:HIS:HB2	49:3R:250:ARG:CG	2.38	0.54
55:4A:129:TYR:OH	55:4A:236:TRP:NE1	2.39	0.54
91:4A:608:PGV:C34	75:4B:302:CDL:H872	2.34	0.54
57:4C:27:MET:HE1	57:4C:50:ASN:ND2	2.23	0.54
75:4C:306:CDL:H142	75:4C:306:CDL:H181	1.88	0.54
75:4C:307:CDL:H392	75:4C:307:CDL:H262	1.90	0.54
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.41	0.53
9:1I:11:SER:OG	9:1I:13:ASP:OD2	2.26	0.53
75:1L:704:CDL:C60	13:1M:371:PRO:HD2	2.38	0.53
13:1M:365:THR:HG21	13:1M:444:LEU:HD21	1.90	0.53
70:1M:501:PC1:H322	75:1i:201:CDL:H172	1.89	0.53
30:1e:27:LYS:HB3	33:1h:138:LYS:HA	1.90	0.53
46:3B:95:LYS:HD3	46:3B:95:LYS:C	2.32	0.53
69:3C:516:3PE:H122	69:3C:516:3PE:H12	1.90	0.53
48:3D:162:PRO:HB2	48:3Q:99:GLU:HG3	1.90	0.53
75:3F:201:CDL:H421	75:3F:201:CDL:C38	2.38	0.53
51:3G:33:THR:HG22	69:3G:103:3PE:C2	2.24	0.53
53:3J:41:ASP:O	53:3J:45:GLU:HG3	2.08	0.53
69:3N:501:3PE:H2D1	75:3N:502:CDL:H601	1.90	0.53
1:1A:19:LEU:O	1:1A:23:TRP:HB2	2.09	0.53
5:1E:159:ASN:HB2	5:1E:184:PRO:HB3	1.89	0.53
7:1G:243:ARG:HB3	7:1G:248:MET:HE3	1.90	0.53
7:1G:524:LEU:HD13	7:1G:543:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:42:LEU:HD22	13:1M:453:MET:HB3	1.91	0.53
16:1P:99:TRP:HZ2	16:1P:276:GLU:HG3	1.70	0.53
27:1b:62:MET:HE3	27:1b:65:VAL:HG21	1.91	0.53
69:1d:201:3PE:C2H	69:1d:201:3PE:C3E	2.73	0.53
31:1f:10:HIS:ND1	69:1f:102:3PE:H252	2.24	0.53
31:1f:22:PHE:CZ	69:1f:104:3PE:C35	2.91	0.53
47:3C:371:ILE:HD11	69:3C:506:3PE:H251	1.89	0.53
50:3F:31:TRP:CH2	75:3F:201:CDL:H762	2.43	0.53
69:3G:109:3PE:H2A1	69:3G:110:3PE:H3B2	1.89	0.53
69:3T:103:3PE:O14	69:3T:103:3PE:H2G1	2.08	0.53
1:1A:18:VAL:HG22	8:1H:222:MET:HG3	1.89	0.53
6:1F:96:ASN:OD1	73:1F:501:FMN:N3	2.42	0.53
7:1G:215:PHE:HB3	9:1I:104:ARG:HG3	1.88	0.53
12:1L:601:LEU:HG	12:1L:602:PHE:CD1	2.43	0.53
29:1d:27:THR:HG21	69:1f:104:3PE:O14	2.08	0.53
34:1i:46:TRP:HE3	34:1i:50:LEU:HB2	1.73	0.53
45:3A:146:ARG:HA	45:3A:149:VAL:HG12	1.89	0.53
46:3B:29:LEU:HB2	46:3B:31:ASN:OD1	2.08	0.53
46:3B:334:GLY:O	46:3B:338:LYS:HD3	2.07	0.53
69:3D:502:3PE:H392	69:3J:101:3PE:H261	1.89	0.53
46:3O:353:SER:O	46:3O:357:VAL:HG23	2.09	0.53
47:3P:156:ILE:HD13	69:3P:507:3PE:C29	2.38	0.53
70:3P:509:PC1:H322	69:3P:514:3PE:H262	1.90	0.53
49:3R:234:TYR:HB2	49:3R:243:TYR:CD2	2.43	0.53
55:4A:253:MET:HG2	55:4A:396:TRP:HZ3	1.72	0.53
93:4B:303:PSC:H201	63:4I:17:LEU:HB3	1.89	0.53
67:4M:34:LEU:HA	67:4M:37:LEU:HG	1.90	0.53
1:1A:38:GLU:HB2	1:1A:43:PRO:HG3	1.89	0.53
7:1G:27:LEU:HD21	7:1G:39:ARG:NH2	2.22	0.53
8:1H:267:THR:O	8:1H:271:LEU:HG	2.09	0.53
8:1H:299:ALA:HB1	27:1b:24:ILE:HB	1.90	0.53
12:1L:601:LEU:HG	12:1L:602:PHE:HD1	1.73	0.53
69:1Y:205:3PE:H2B1	70:1Y:206:PC1:H3E1	1.90	0.53
69:1d:201:3PE:H2I1	75:1d:202:CDL:H461	1.91	0.53
34:1i:83:TYR:CG	75:1i:201:CDL:H531	2.44	0.53
39:1n:64:ARG:NH2	39:1n:67:GLU:OE1	2.27	0.53
69:3A:503:3PE:H111	75:3Y:106:CDL:C51	2.36	0.53
49:3E:182:LYS:HD3	49:3E:183:GLU:N	2.23	0.53
75:3F:201:CDL:H451	69:3G:110:3PE:H381	1.89	0.53
45:3N:358:LYS:O	45:3N:362:ARG:HG3	2.08	0.53
49:3R:83:ILE:HG13	49:3R:83:ILE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:126:ALA:HB2	69:3R:304:3PE:H2H2	1.91	0.53
49:3R:181:LYS:O	49:3R:184:ILE:N	2.42	0.53
69:3S:201:3PE:H392	70:3T:102:PC1:C26	2.39	0.53
53:3W:9:ARG:HD3	53:3W:9:ARG:N	2.23	0.53
53:3W:34:ARG:HG2	54:3X:47:TYR:CE2	2.44	0.53
7:1G:272:ASP:OD2	7:1G:683:THR:OG1	2.26	0.53
75:1L:704:CDL:H152	69:1L:709:3PE:H241	1.89	0.53
20:1T:14:ARG:HD2	20:1T:17:TYR:HE2	1.73	0.53
70:1Y:202:PC1:H252	69:1m:201:3PE:H382	1.91	0.53
75:1Y:217:CDL:H611	75:1Y:217:CDL:C43	2.38	0.53
75:1g:201:CDL:OB9	33:1h:30:LEU:HB2	2.08	0.53
69:1h:204:3PE:H11	69:1h:204:3PE:H232	1.89	0.53
34:1i:39:VAL:HG12	34:1i:44:GLN:HG3	1.90	0.53
37:1l:16:THR:OG1	37:1l:18:GLU:OE1	2.21	0.53
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.17	0.53
37:1l:115:MET:HA	37:1l:118:VAL:HG12	1.88	0.53
37:1l:121:ILE:HG13	37:1l:122:TYR:HD1	1.73	0.53
44:1s:58:LEU:HD23	44:1s:61:PHE:HE1	1.73	0.53
47:3C:299:LEU:HD12	69:3C:512:3PE:C3I	2.36	0.53
50:3F:86:ILE:HD12	50:3F:92:TRP:CZ2	2.44	0.53
69:3P:511:3PE:C3A	69:3P:512:3PE:H392	2.25	0.53
57:4C:27:MET:HE1	57:4C:50:ASN:HD22	1.74	0.53
60:4F:53:THR:HG22	60:4F:54:ASN:H	1.74	0.53
62:4H:14:ALA:HB3	62:4H:63:PHE:CE1	2.42	0.53
4:1D:177:MET:HE3	4:1D:214:PHE:CE2	2.44	0.53
5:1E:194:GLU:HG2	6:1F:28:ARG:HH21	1.73	0.53
7:1G:43:HIS:HB3	7:1G:46:LEU:HB2	1.90	0.53
7:1G:620:ARG:NH1	7:1G:633:TYR:OH	2.42	0.53
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.89	0.53
15:1O:53:GLU:HG2	15:1O:104:ARG:HH12	1.73	0.53
20:1T:72:CYS:HB2	20:1T:75:GLU:HG3	1.89	0.53
23:1X:154:GLU:OE1	23:1X:154:GLU:N	2.42	0.53
24:1Y:38:TYR:HE2	69:1Y:204:3PE:H392	1.74	0.53
75:1Y:217:CDL:H551	75:1Y:217:CDL:H772	1.90	0.53
69:1d:201:3PE:C2I	75:1d:202:CDL:H461	2.39	0.53
75:1g:201:CDL:C11	69:1g:203:3PE:H231	2.38	0.53
46:3B:227:ARG:HG3	46:3B:229:GLY:N	2.24	0.53
47:3C:109:PHE:HB3	47:3C:112:THR:CG2	2.39	0.53
47:3C:363:LEU:HD12	69:3C:512:3PE:H2H2	1.91	0.53
69:3N:501:3PE:H2C1	75:3N:502:CDL:H551	1.90	0.53
46:3O:45:SER:HB3	46:3O:116:ILE:HG13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:117:GLU:O	46:3O:121:GLU:HG2	2.08	0.53
47:3P:92:ILE:CD1	69:3P:519:3PE:H2B1	2.39	0.53
47:3P:342:PRO:HB2	47:3P:344:GLU:CG	2.37	0.53
69:3P:510:3PE:H3C2	69:3P:517:3PE:H2I2	1.89	0.53
48:3Q:3:LEU:HD11	52:3U:56:GLU:HG2	1.90	0.53
48:3Q:138:PRO:O	48:3Q:139:THR:C	2.52	0.53
48:3Q:210:MET:HE1	53:3W:40:ALA:HB1	1.89	0.53
50:3S:19:TRP:CZ3	69:3S:201:3PE:H351	2.43	0.53
75:3X:103:CDL:H231	69:3X:105:3PE:H3H2	1.91	0.53
55:4A:142:SER:O	55:4A:146:THR:HG23	2.09	0.53
93:4B:303:PSC:C20	63:4I:18:ARG:HG3	2.35	0.53
4:1D:357:GLN:O	43:1r:59:ARG:NH1	2.41	0.53
10:1J:87:LYS:HB2	69:1J:201:3PE:O14	2.08	0.53
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.90	0.53
20:1U:18:VAL:HB	20:1U:54:MET:HE1	1.91	0.53
22:1W:22:SER:OG	22:1W:31:ARG:NH2	2.39	0.53
69:1Y:215:3PE:H271	69:1Y:215:3PE:H381	1.90	0.53
31:1f:18:VAL:HG21	69:1f:101:3PE:H3C1	1.90	0.53
75:1g:201:CDL:H772	33:1h:34:ILE:HG22	1.90	0.53
47:3C:158:THR:O	47:3C:161:VAL:HG12	2.08	0.53
47:3C:244:LEU:HD12	48:3D:297:MET:HE2	1.90	0.53
69:3C:511:3PE:H362	69:3C:512:3PE:H282	1.90	0.53
52:3H:55:CYS:HB3	52:3H:86:PHE:CE1	2.44	0.53
49:3I:55:LEU:O	49:3I:56:SER:C	2.51	0.53
45:3N:121:SER:HB2	45:3N:123:GLU:HG2	1.90	0.53
70:3P:509:PC1:H351	69:3P:514:3PE:H3D1	1.89	0.53
69:3P:510:3PE:H2A2	69:3P:510:3PE:H262	1.90	0.53
55:4A:299:VAL:HG23	62:4H:22:ASN:OD1	2.08	0.53
57:4C:76:GLN:O	57:4C:80:ARG:HG3	2.09	0.53
1:1A:83:ASN:OD1	70:1J:202:PC1:H153	2.09	0.53
2:1B:47:PRO:HD2	2:1B:75:VAL:O	2.08	0.53
75:1H:401:CDL:HB61	75:1H:401:CDL:C33	2.38	0.53
12:1L:24:SER:HB2	69:1L:710:3PE:H2	1.91	0.53
13:1M:29:VAL:HG21	69:1g:202:3PE:C29	2.39	0.53
14:1N:170:LEU:O	14:1N:295:ARG:NH2	2.40	0.53
14:1N:324:LYS:CG	75:1d:205:CDL:HA32	2.38	0.53
23:1X:168:PHE:CZ	75:1d:202:CDL:H172	2.43	0.53
24:1Y:32:GLY:HA2	24:1Y:35:VAL:HG13	1.88	0.53
69:1Y:209:3PE:H3A1	69:1Y:213:3PE:H2A2	1.90	0.53
75:1g:201:CDL:H621	75:1g:201:CDL:H762	1.91	0.53
47:3C:82:LEU:HD12	47:3C:243:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3J:39:GLY:HA3	69:3J:104:3PE:C3A	2.39	0.53
48:3Q:207:LYS:HA	48:3Q:210:MET:CE	2.38	0.53
52:3U:50:THR:HG22	52:3U:51:GLU:N	2.23	0.53
53:3W:56:ILE:C	53:3W:57:LYS:CG	2.59	0.53
54:3Y:10:TYR:CD1	75:3Y:106:CDL:H331	2.44	0.53
55:4A:62:ALA:HB2	88:4A:601:HEA:HBD1	1.91	0.53
55:4A:350:VAL:HG13	75:4B:302:CDL:H622	1.91	0.53
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.44	0.53
13:1M:122:PHE:HE2	13:1M:206:LYS:HD3	1.73	0.53
13:1M:127:VAL:HB	13:1M:128:PRO:HD3	1.91	0.53
14:1N:209:ILE:HD12	75:1N:402:CDL:H602	1.88	0.53
69:1Z:201:3PE:H222	43:1r:13:TRP:HZ2	1.74	0.53
46:3B:129:ALA:N	46:3B:130:PRO:HD3	2.24	0.53
47:3C:285:PRO:HD2	69:3C:512:3PE:H222	1.91	0.53
69:3C:508:3PE:H2E1	69:3C:508:3PE:C3A	2.39	0.53
69:3N:501:3PE:H2G2	70:3X:104:PC1:H3G2	1.91	0.53
54:3Y:13:LEU:HB3	75:3Y:106:CDL:H141	1.89	0.53
57:4C:204:HIS:O	57:4C:208:VAL:HG23	2.09	0.53
91:4G:102:PGV:H211	91:4G:102:PGV:H92	1.90	0.53
1:1A:23:TRP:O	70:1A:202:PC1:H142	2.08	0.53
2:1B:38:ASN:O	2:1B:42:ARG:HG2	2.08	0.53
4:1D:165:THR:HG23	8:1H:32:GLN:HG2	1.91	0.53
9:1I:54:LYS:HD2	42:1q:90:LEU:HD23	1.91	0.53
12:1L:526:LEU:HD12	12:1L:530:PRO:HG2	1.90	0.53
12:1L:603:ASN:HB2	69:1L:706:3PE:C11	2.39	0.53
69:1L:703:3PE:H341	69:1o:201:3PE:H3C2	1.91	0.53
13:1M:127:VAL:HG11	69:1N:401:3PE:C3F	2.39	0.53
14:1N:26:TRP:CE2	14:1N:86:ILE:HG12	2.44	0.53
16:1P:45:VAL:HB	16:1P:68:ILE:HG13	1.89	0.53
24:1Y:109:ILE:HG23	70:1Y:206:PC1:C35	2.39	0.53
25:1Z:83:VAL:HG22	25:1Z:124:LEU:HD21	1.90	0.53
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.09	0.53
75:1i:201:CDL:H561	41:1p:44:VAL:HA	1.91	0.53
49:3E:156:LEU:O	49:3E:158:ASP:N	2.42	0.53
49:3E:206:LYS:NZ	49:3E:264:GLU:HA	2.24	0.53
69:3J:103:3PE:H11	69:3J:103:3PE:O22	2.09	0.53
45:3N:188:GLN:O	45:3N:223:TYR:HE1	1.92	0.53
69:3N:501:3PE:H2I3	70:3X:104:PC1:H3F1	1.90	0.53
46:3O:56:ARG:HA	46:3O:171:ALA:O	2.09	0.53
47:3P:323:CYS:HB2	69:3P:516:3PE:H3H1	1.91	0.53
49:3R:183:GLU:H	49:3R:183:GLU:CD	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:144:ASP:OD2	57:4C:36:HIS:NE2	2.41	0.53
4:1D:291:GLY:O	4:1D:296:ARG:NH2	2.43	0.52
12:1L:24:SER:C	69:1L:710:3PE:O14	2.52	0.52
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.08	0.52
20:1U:13:ASP:O	20:1U:17:TYR:HB2	2.09	0.52
69:1Y:209:3PE:H362	69:1Y:213:3PE:H251	1.90	0.52
69:1d:201:3PE:H31	69:1d:201:3PE:H262	1.91	0.52
70:1h:202:PC1:H2C2	69:1h:204:3PE:H3F1	1.91	0.52
40:1o:51:MET:HB2	40:1o:54:GLN:HG3	1.92	0.52
45:3A:269:PRO:HB2	45:3A:410:VAL:HG11	1.90	0.52
45:3A:349:ALA:CB	45:3A:408:ARG:HG3	2.40	0.52
46:3B:250:ASP:O	46:3B:251:SER:C	2.49	0.52
69:3C:515:3PE:H3A2	69:3C:516:3PE:H361	1.91	0.52
48:3D:139:LEU:HD11	48:3D:179:PHE:CZ	2.44	0.52
48:3D:147:GLU:H	48:3D:147:GLU:CD	2.15	0.52
69:3G:108:3PE:H361	69:3G:108:3PE:H271	1.91	0.52
69:3G:110:3PE:H292	69:3G:110:3PE:H2D1	1.90	0.52
53:3J:43:ILE:HG12	69:3J:104:3PE:H331	1.91	0.52
45:3N:358:LYS:CD	45:3N:402:VAL:HG13	2.39	0.52
47:3P:304:MET:N	47:3P:305:PRO:HD2	2.24	0.52
47:3P:330:ALA:HB3	69:3P:510:3PE:H2G2	1.91	0.52
69:3P:503:3PE:H2H2	69:3P:518:3PE:C3H	2.38	0.52
69:3P:510:3PE:H2F2	51:3T:54:VAL:HG22	1.91	0.52
69:3P:511:3PE:O12	75:3X:103:CDL:H531	2.09	0.52
49:3R:264:GLU:HB2	49:3R:272:ILE:HG12	1.91	0.52
69:3R:302:3PE:H3D2	70:3R:303:PC1:H391	1.90	0.52
6:1F:253:THR:OG1	6:1F:269:GLU:OE2	2.18	0.52
6:1F:256:PHE:CG	6:1F:279:LEU:HD21	2.44	0.52
8:1H:140:ILE:HA	8:1H:143:GLU:HG3	1.90	0.52
10:1J:99:MET:HE1	69:1J:201:3PE:C3E	2.39	0.52
13:1M:263:MET:HE3	38:1m:101:TYR:HA	1.90	0.52
14:1N:11:MET:HG2	75:1N:402:CDL:C18	2.39	0.52
14:1N:179:MET:HE1	14:1N:251:MET:HE1	1.91	0.52
14:1N:324:LYS:HG3	75:1d:205:CDL:HA32	1.90	0.52
15:1O:169:VAL:HG21	15:1O:214:MET:HG2	1.91	0.52
16:1P:270:PHE:CE2	16:1P:278:TRP:HE3	2.25	0.52
43:1r:51:ASN:O	43:1r:56:ARG:NH2	2.43	0.52
47:3C:245:PHE:HB3	69:3C:504:3PE:H332	1.91	0.52
49:3E:187:GLU:HA	49:3E:190:VAL:CG2	2.40	0.52
45:3N:414:TYR:O	45:3N:418:GLN:HG3	2.08	0.52
48:3Q:15:ARG:CD	69:3Q:504:3PE:O12	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:234:TYR:HB2	49:3R:243:TYR:HB2	1.91	0.52
56:4B:160:LEU:HD11	56:4B:175:ILE:HG23	1.89	0.52
75:4C:306:CDL:H761	75:4C:306:CDL:H612	1.91	0.52
75:4C:307:CDL:H341	75:4C:307:CDL:H192	1.89	0.52
2:1B:176:TRP:CE3	70:1B:202:PC1:C26	2.92	0.52
8:1H:9:LEU:HD12	26:1a:19:PRO:HB3	1.90	0.52
8:1H:90:PRO:HD2	8:1H:240:ILE:HD13	1.92	0.52
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.91	0.52
12:1L:500:LEU:HD12	64:4J:30:ILE:HG13	1.91	0.52
13:1M:1:FME:SD	13:1M:111:THR:HG21	2.49	0.52
24:1Y:108:GLY:HA3	70:1Y:206:PC1:H31	1.92	0.52
75:3A:501:CDL:H352	69:3A:503:3PE:H3C2	1.92	0.52
69:3A:503:3PE:H122	69:3C:516:3PE:HN2	1.74	0.52
46:3B:308:ASP:N	46:3B:327:ILE:O	2.42	0.52
48:3D:139:LEU:HD11	48:3D:179:PHE:HZ	1.71	0.52
48:3D:193:ASN:HB2	48:3D:196:ALA:O	2.09	0.52
49:3E:255:PRO:O	49:3E:256:LEU:HB3	2.08	0.52
51:3G:56:VAL:O	51:3G:60:VAL:HG13	2.08	0.52
70:3J:106:PC1:H2F1	69:3P:507:3PE:C3I	2.38	0.52
47:3P:75:TYR:HD2	49:3R:138:SER:HG	1.57	0.52
69:3R:305:3PE:H3I1	69:3T:103:3PE:C38	2.30	0.52
56:4B:181:GLN:H	62:4H:23:GLN:HG3	1.74	0.52
87:4G:103:PEK:H11	87:4G:103:PEK:H272	1.92	0.52
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.90	0.52
4:1D:373:GLU:OE1	4:1D:392:LYS:NZ	2.42	0.52
7:1G:359:ARG:NH1	7:1G:504:ASP:OD2	2.43	0.52
12:1L:563:PRO:O	12:1L:566:THR:HG22	2.10	0.52
12:1L:573:MET:HG2	14:1N:167:TRP:CZ2	2.45	0.52
13:1M:153:THR:HG22	13:1M:206:LYS:HZ3	1.74	0.52
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.45	0.52
18:1R:49:VAL:HG22	18:1R:90:GLN:HB2	1.92	0.52
24:1Y:87:LEU:HD11	69:1Y:212:3PE:H332	1.84	0.52
75:1d:202:CDL:H273	75:1d:202:CDL:C34	2.39	0.52
45:3A:172:GLU:CD	45:3A:172:GLU:H	2.17	0.52
49:3E:181:LYS:HA	49:3E:184:ILE:CG2	2.40	0.52
75:3F:201:CDL:H1	75:3F:201:CDL:CA5	2.40	0.52
46:3O:169:ARG:CG	46:3O:240:ARG:HB3	2.36	0.52
93:4B:303:PSC:H083	63:4I:14:ALA:CB	2.39	0.52
69:1A:203:3PE:H232	14:1N:2:ASN:HD21	1.74	0.52
5:1E:78:MET:HA	5:1E:81:TYR:CD2	2.45	0.52
6:1F:361:GLN:O	7:1G:51:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:2:PHE:O	8:1H:6:ILE:HG13	2.09	0.52
8:1H:54:LYS:HZ1	8:1H:55:LEU:HA	1.75	0.52
9:1I:86:VAL:O	9:1I:87:CYS:C	2.52	0.52
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.10	0.52
13:1M:95:TYR:HD1	13:1M:136:TRP:CE3	2.28	0.52
14:1N:133:TRP:CE3	75:1N:402:CDL:H591	2.42	0.52
69:1N:401:3PE:H221	69:1d:201:3PE:O32	2.09	0.52
15:1O:310:GLU:HA	15:1O:314:ASP:HB2	1.90	0.52
26:1a:7:PRO:HD3	75:1q:201:CDL:H172	1.91	0.52
34:1i:99:ARG:HA	41:1p:115:ARG:HA	1.91	0.52
69:1m:205:3PE:H31	69:1m:205:3PE:H231	1.92	0.52
69:3D:502:3PE:H272	69:3J:101:3PE:H2A2	1.92	0.52
49:3I:58:GLN:O	49:3I:59:ALA:C	2.53	0.52
53:3J:53:TRP:O	53:3J:54:LYS:CB	2.58	0.52
53:3J:59:LYS:N	53:3J:60:TYR:N	2.39	0.52
46:3O:181:TYR:CZ	46:3O:182:ARG:HG2	2.45	0.52
47:3P:337:TRP:CH2	51:3T:59:TYR:HA	2.44	0.52
48:3Q:8:PRO:HG2	48:3Q:10:TYR:CE1	2.45	0.52
69:3W:101:3PE:H251	69:3W:102:3PE:H31	1.90	0.52
55:4A:265:LYS:HB3	55:4A:490:THR:HG21	1.90	0.52
1:1A:23:TRP:NE1	70:1A:202:PC1:O21	2.27	0.52
4:1D:238:ARG:NH2	4:1D:412:ALA:HB1	2.25	0.52
5:1E:174:ASP:OD1	5:1E:175:GLU:N	2.42	0.52
7:1G:41:CYS:O	7:1G:161:ARG:NH1	2.41	0.52
8:1H:189:THR:HG22	8:1H:270:PHE:HZ	1.73	0.52
9:1I:78:ILE:HG21	18:1R:86:TYR:HA	1.91	0.52
12:1L:316:THR:HA	12:1L:319:ILE:HG12	1.92	0.52
13:1M:306:PRO:HA	13:1M:458:LEU:HD22	1.92	0.52
15:1O:38:LEU:O	15:1O:41:GLU:N	2.43	0.52
16:1P:108:ASP:OD1	16:1P:108:ASP:N	2.42	0.52
69:1Y:205:3PE:H232	69:1Y:208:3PE:H232	1.90	0.52
69:1Y:215:3PE:C3D	47:3P:357:LEU:HD21	2.40	0.52
31:1f:25:TYR:OH	69:1f:104:3PE:C21	2.57	0.52
69:1f:101:3PE:C39	69:1f:101:3PE:H351	2.40	0.52
46:3B:83:PHE:CE2	46:3B:87:ARG:HG3	2.45	0.52
46:3B:243:GLU:HB2	46:3B:436:VAL:HG21	1.90	0.52
46:3B:278:VAL:HG13	46:3B:356:ASP:OD2	2.08	0.52
47:3C:221:HIS:O	47:3C:225:THR:OG1	2.21	0.52
69:3C:507:3PE:H2F2	69:3G:109:3PE:H3B1	1.91	0.52
49:3I:67:SER:O	49:3I:74:ALA:HA	2.10	0.52
48:3Q:18:LEU:HD22	48:3Q:206:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3Q:502:3PE:O12	69:3Q:504:3PE:H221	2.10	0.52
49:3R:207:LYS:O	49:3R:208:PRO:C	2.51	0.52
51:3T:34:ILE:HB	51:3T:35:PRO:HD3	1.92	0.52
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	1.92	0.52
10:1J:46:ASN:O	10:1J:128:TYR:OH	2.23	0.52
12:1L:24:SER:HA	69:1L:710:3PE:O11	2.10	0.52
69:1L:702:3PE:C29	34:1i:80:ILE:HG23	2.37	0.52
13:1M:197:LEU:CB	82:1Y:203:PGT:H411	2.27	0.52
69:1M:502:3PE:H271	69:1M:502:3PE:O32	2.10	0.52
75:1d:202:CDL:H341	75:1d:202:CDL:H572	1.90	0.52
34:1i:83:TYR:CD2	75:1i:201:CDL:C51	2.86	0.52
40:1o:75:ASN:ND2	69:1o:201:3PE:O22	2.43	0.52
45:3A:145:MET:HE3	45:3A:425:LEU:HG	1.92	0.52
46:3B:70:ARG:O	49:3I:68:VAL:HG21	2.09	0.52
46:3B:359:ALA:O	46:3B:363:LYS:HG3	2.10	0.52
49:3E:184:ILE:O	49:3E:188:ALA:N	2.24	0.52
49:3E:238:CYS:O	48:3Q:147:LEU:HD21	2.10	0.52
69:3G:109:3PE:O14	69:3G:109:3PE:N	2.42	0.52
45:3N:223:TYR:CD2	45:3N:228:VAL:HB	2.44	0.52
48:3Q:174:GLY:O	48:3Q:175:THR:C	2.51	0.52
49:3R:205:VAL:HG22	49:3R:207:LYS:C	2.35	0.52
49:3R:242:HIS:CE1	49:3R:251:LYS:HE3	2.44	0.52
69:3R:302:3PE:H3A2	69:3R:302:3PE:H3E2	1.92	0.52
69:3S:201:3PE:H32	69:3S:201:3PE:C23	2.25	0.52
55:4A:419:VAL:HA	91:4A:608:PGV:H142	1.91	0.52
3:1C:83:VAL:HG12	3:1C:85:THR:HG22	1.90	0.52
4:1D:339:LYS:HB3	18:1R:69:PRO:HA	1.92	0.52
6:1F:426:LEU:O	6:1F:430:MET:HG3	2.10	0.52
7:1G:116:LEU:HG	7:1G:154:ILE:HD13	1.90	0.52
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.92	0.52
7:1G:324:ASP:OD1	7:1G:324:ASP:N	2.40	0.52
24:1Y:27:ILE:HG21	69:1Y:208:3PE:C2F	2.39	0.52
70:1Y:206:PC1:H291	70:1Y:207:PC1:H2E1	1.92	0.52
25:1Z:138:TYR:HD2	25:1Z:142:TRP:CZ2	2.28	0.52
75:1q:202:CDL:H121	75:1q:202:CDL:H722	1.92	0.52
45:3A:118:GLN:NE2	45:3A:216:PHE:HA	2.21	0.52
46:3B:109:VAL:HB	46:3B:119:LEU:HD12	1.90	0.52
46:3B:123:LEU:O	46:3B:126:VAL:HG22	2.10	0.52
48:3D:150:LYS:HG3	48:3D:175:LEU:HG	1.91	0.52
48:3D:254:TYR:CZ	48:3D:257:VAL:HG23	2.45	0.52
69:3J:104:3PE:H2I2	69:3J:105:3PE:H372	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:70:ARG:O	45:3N:71:PRO:C	2.52	0.52
47:3P:30:TRP:NE1	69:3P:508:3PE:O22	2.43	0.52
49:3R:248:ARG:HH11	49:3R:257:ASN:HB3	1.75	0.52
69:3W:101:3PE:H11	69:3W:101:3PE:C11	2.39	0.52
54:3Y:6:LEU:O	54:3Y:10:TYR:HD2	1.93	0.52
58:4D:118:LYS:HE3	65:4K:53:TRP:HA	1.92	0.52
4:1D:299:CYS:O	4:1D:303:GLU:HG2	2.10	0.52
9:1I:66:ALA:HB1	9:1I:158:GLY:CA	2.39	0.52
10:1J:99:MET:HG3	69:1J:201:3PE:C3I	2.40	0.52
11:1K:85:TYR:CD2	11:1K:92:ASN:HB3	2.44	0.52
12:1L:504:LEU:CD1	69:1L:707:3PE:HN1	2.22	0.52
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	1.92	0.52
24:1Y:98:LEU:HD22	70:1Y:207:PC1:H241	1.91	0.52
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.10	0.52
40:1o:76:PHE:CE1	69:1o:201:3PE:H2B1	2.43	0.52
41:1p:105:ILE:HG13	41:1p:134:VAL:HG21	1.91	0.52
46:3B:341:TYR:O	46:3B:345:LYS:HG3	2.10	0.52
47:3C:181:PHE:HE1	47:3P:53:MET:HE2	1.74	0.52
47:3C:353:LEU:HD22	69:3C:511:3PE:H2F2	1.92	0.52
69:3C:512:3PE:O11	69:3C:513:3PE:H222	2.09	0.52
47:3P:15:ASN:HA	47:3P:19:ILE:HD12	1.91	0.52
47:3P:333:ILE:HG23	69:3P:519:3PE:H341	1.90	0.52
55:4A:230:LEU:HB2	57:4C:103:HIS:NE2	2.25	0.52
91:4A:607:PGV:H22	68:4N:1:MET:HG3	1.92	0.52
57:4C:58:TRP:HD1	57:4C:61:ILE:HD12	1.74	0.52
91:4C:302:PGV:H311	75:4C:307:CDL:H421	1.92	0.52
59:4E:63:SER:O	59:4E:67:ILE:HG23	2.09	0.52
60:4F:21:MET:O	60:4F:25:ARG:HG2	2.10	0.52
4:1D:342:MET:SD	7:1G:101:HIS:HD2	2.33	0.52
6:1F:292:ASP:O	6:1F:339:ARG:NH1	2.43	0.52
7:1G:135:ARG:NH2	7:1G:155:GLN:HE22	2.08	0.52
12:1L:214:ILE:HG21	69:1L:711:3PE:C37	2.40	0.52
24:1Y:79:VAL:HB	69:1Y:214:3PE:H222	1.92	0.52
24:1Y:98:LEU:HD11	69:1Y:212:3PE:C2F	2.40	0.52
25:1Z:110:VAL:HG13	30:1e:70:LYS:HE2	1.92	0.52
69:1e:201:3PE:H381	69:1e:201:3PE:H2F2	1.91	0.52
42:1q:9:ARG:NH1	75:1q:201:CDL:OA3	2.43	0.52
46:3B:117:GLU:HG3	46:3B:118:ILE:N	2.25	0.52
46:3B:385:GLN:HG2	46:3B:391:SER:O	2.10	0.52
47:3C:357:LEU:O	47:3C:361:ILE:HG13	2.10	0.52
50:3F:55:VAL:O	50:3F:59:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:3H:53:GLU:HA	52:3H:56:ILE:HB	1.92	0.52
75:3N:502:CDL:H151	75:3N:502:CDL:H561	1.91	0.52
47:3P:361:ILE:HA	47:3P:365:LEU:HB2	1.91	0.52
47:3P:371:ILE:HD11	69:3P:506:3PE:H252	1.92	0.52
69:3P:504:3PE:H382	69:3Y:103:3PE:H271	1.92	0.52
55:4A:418:PHE:HE2	91:4A:608:PGV:H101	1.75	0.52
69:1B:204:3PE:H2D2	69:1B:204:3PE:C2H	2.38	0.51
4:1D:29:LYS:HG2	4:1D:30:PRO:HD2	1.92	0.51
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.26	0.51
10:1J:170:GLU:HA	10:1J:170:GLU:OE1	2.10	0.51
12:1L:78:LEU:HD11	75:1L:704:CDL:H861	1.91	0.51
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.35	0.51
12:1L:591:PHE:CE1	14:1N:110:PRO:O	2.61	0.51
69:1Y:214:3PE:C2G	69:1Y:216:3PE:H2I1	2.40	0.51
75:1g:201:CDL:H141	33:1h:28:TYR:HE1	1.75	0.51
38:1m:29:ARG:HG3	45:3N:225:GLU:CD	2.35	0.51
45:3A:445:ARG:HH22	75:3A:501:CDL:HB21	1.75	0.51
47:3C:215:MET:HE1	50:3F:74:ILE:HG21	1.91	0.51
47:3C:342:PRO:HB2	47:3C:344:GLU:CG	2.40	0.51
49:3E:195:LEU:HB3	49:3E:250:ARG:O	2.09	0.51
69:3G:111:3PE:H292	69:3G:111:3PE:C23	2.40	0.51
45:3N:192:ALA:HB3	45:3N:193:PRO:HD3	1.92	0.51
75:3N:502:CDL:H311	47:3P:19:ILE:CG1	2.39	0.51
47:3P:171:ASP:CG	47:3P:172:LYS:H	2.18	0.51
48:3Q:210:MET:HE1	53:3W:40:ALA:HB2	1.92	0.51
48:3Q:232:SER:O	48:3Q:234:LYS:HE2	2.10	0.51
69:3T:103:3PE:H2	69:3T:103:3PE:C2E	2.35	0.51
52:3U:20:VAL:HG13	52:3U:72:LYS:HG3	1.92	0.51
52:3U:68:CYS:O	52:3U:72:LYS:HE3	2.10	0.51
68:4N:6:ILE:O	68:4N:10:LYS:HG2	2.11	0.51
68:4N:48:LYS:HD2	68:4N:48:LYS:H	1.75	0.51
6:1F:361:GLN:NE2	17:1Q:133:LYS:NZ	2.58	0.51
10:1J:21:SER:HB3	11:1K:14:ILE:CD1	2.40	0.51
69:1L:708:3PE:H31	69:1L:708:3PE:H222	1.92	0.51
14:1N:238:PRO:CB	69:1N:401:3PE:H11	2.40	0.51
14:1N:270:MET:HB3	14:1N:275:SER:HB3	1.93	0.51
20:1U:17:TYR:O	20:1U:20:LYS:HG2	2.10	0.51
24:1Y:107:TYR:CD2	69:1Y:213:3PE:P	2.90	0.51
69:1d:206:3PE:H382	69:1f:104:3PE:C2A	2.38	0.51
31:1f:31:ASP:O	31:1f:35:THR:HG23	2.10	0.51
45:3A:156:THR:HB	45:3A:241:ILE:CD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:251:ALA:HB1	45:3A:428:ILE:HG22	1.92	0.51
75:3A:501:CDL:H232	69:3A:502:3PE:H381	1.91	0.51
46:3B:109:VAL:HG22	46:3B:123:LEU:HD22	1.92	0.51
49:3E:160:PRO:O	49:3E:163:LYS:HB2	2.10	0.51
51:3G:63:TRP:CZ2	69:3G:110:3PE:H2	2.45	0.51
69:3P:504:3PE:H261	69:3Y:103:3PE:H231	1.91	0.51
49:3R:152:ILE:O	49:3R:153:GLU:HG2	2.09	0.51
49:3R:191:GLU:HB3	49:3R:194:GLN:CD	2.34	0.51
49:3R:195:LEU:HB3	49:3R:248:ARG:NH2	2.25	0.51
75:3X:103:CDL:H371	69:3X:105:3PE:H282	1.93	0.51
69:3X:107:3PE:H321	69:4G:104:3PE:H252	1.92	0.51
56:4B:52:HIS:CD2	59:4E:40:ASP:HB2	2.45	0.51
56:4B:59:GLN:NE2	68:4N:13:PRO:HD2	2.25	0.51
62:4H:5:GLN:HG3	62:4H:6:THR:HG23	1.92	0.51
2:1B:77:ARG:HG3	2:1B:78:ALA:H	1.74	0.51
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.92	0.51
8:1H:262:LYS:HG2	70:1H:404:PC1:H341	1.92	0.51
11:1K:44:SER:HB3	11:1K:59:MET:HE1	1.92	0.51
12:1L:23:ASN:HB2	69:1L:709:3PE:P	2.50	0.51
69:1L:709:3PE:C2A	13:1M:446:LEU:HD11	2.30	0.51
69:1L:710:3PE:C21	33:1h:26:ARG:NH1	2.69	0.51
13:1M:6:ILE:CD1	31:1f:26:LEU:HD12	2.41	0.51
13:1M:328:CYS:HB3	13:1M:437:MET:HE1	1.92	0.51
14:1N:346:LEU:HD11	70:1d:204:PC1:H3B1	1.93	0.51
24:1Y:107:TYR:CE2	69:1Y:213:3PE:H112	2.45	0.51
34:1i:39:VAL:O	34:1i:44:GLN:NE2	2.42	0.51
46:3B:291:ALA:C	46:3B:293:SER:H	2.19	0.51
47:3C:284:ILE:CD1	69:3C:512:3PE:C35	2.48	0.51
69:3C:505:3PE:H2C1	69:3C:505:3PE:H391	1.92	0.51
49:3E:155:LYS:HD2	49:3E:176:VAL:HG11	1.92	0.51
49:3E:236:CYS:HB2	49:3E:241:SER:O	2.11	0.51
45:3N:442:PHE:CE1	69:3N:503:3PE:H121	2.45	0.51
45:3N:445:ARG:HH11	75:3X:103:CDL:HB61	1.74	0.51
46:3O:319:SER:OG	46:3O:320:GLY:N	2.43	0.51
49:3R:178:HIS:O	49:3R:179:ARG:C	2.52	0.51
69:3W:102:3PE:H3A2	69:3X:101:3PE:H3B2	1.92	0.51
4:1D:18:VAL:HG22	14:1N:171:ASN:OD1	2.10	0.51
6:1F:338:ASP:OD1	6:1F:341:THR:OG1	2.29	0.51
8:1H:102:VAL:HG11	8:1H:154:LEU:HD11	1.92	0.51
10:1J:99:MET:CE	69:1J:201:3PE:C3I	2.39	0.51
69:1J:203:3PE:H3B2	69:1J:203:3PE:H2A1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:310:ASN:HD21	15:1O:98:SER:HB3	1.75	0.51
75:1N:402:CDL:H161	69:1e:201:3PE:C32	2.40	0.51
15:1O:132:PHE:CZ	15:1O:210:PHE:HB2	2.46	0.51
23:1X:171:MET:HE3	29:1d:30:ARG:NE	2.25	0.51
24:1Y:80:ARG:CG	69:1Y:214:3PE:O14	2.41	0.51
69:1Y:215:3PE:H342	69:3P:510:3PE:C3D	2.41	0.51
25:1Z:140:PHE:HD1	26:1a:45:TRP:HB2	1.75	0.51
26:1a:44:GLN:HA	26:1a:47:LEU:HD12	1.92	0.51
69:1d:206:3PE:H381	69:1f:104:3PE:C2C	2.37	0.51
69:1f:102:3PE:H331	69:1g:203:3PE:H371	1.92	0.51
69:1l:202:3PE:H291	69:1l:203:3PE:H352	1.91	0.51
40:1o:17:ASP:HB3	40:1o:20:ARG:HG2	1.93	0.51
45:3A:445:ARG:HH12	69:3A:503:3PE:H2	1.75	0.51
46:3B:203:ARG:HD2	46:3B:230:LEU:O	2.09	0.51
47:3C:108:MET:HA	47:3C:108:MET:HE3	1.91	0.51
45:3N:79:VAL:HA	45:3N:82:MET:HE2	1.92	0.51
45:3N:356:ARG:HG2	45:3N:360:ILE:HD11	1.93	0.51
47:3P:141:TRP:CD1	47:3P:265:PRO:CD	2.93	0.51
69:3P:507:3PE:H2H1	69:3Y:104:3PE:H3C1	1.92	0.51
53:3W:58:HIS:HB2	53:3W:59:LYS:HG3	1.92	0.51
56:4B:90:ILE:HD12	56:4B:183:THR:HB	1.92	0.51
57:4C:58:TRP:CE2	91:4C:305:PGV:H61	2.45	0.51
57:4C:107:ALA:HB1	68:4N:42:ASP:HB3	1.93	0.51
68:4N:2:LEU:CD1	68:4N:2:LEU:N	2.67	0.51
68:4N:33:VAL:CG2	91:4N:101:PGV:H41	2.40	0.51
6:1F:362:CYS:SG	6:1F:404:ILE:HG23	2.51	0.51
13:1M:259:TYR:N	13:1M:260:PRO:HD2	2.26	0.51
14:1N:337:LEU:HD23	75:1d:202:CDL:H191	1.93	0.51
24:1Y:98:LEU:HD21	70:1Y:207:PC1:H272	1.91	0.51
69:1d:206:3PE:C35	69:1f:104:3PE:H292	2.40	0.51
33:1h:77:ARG:NH2	69:1h:204:3PE:O31	2.43	0.51
70:1h:202:PC1:H391	69:1h:204:3PE:C36	2.40	0.51
35:1j:38:TRP:CZ2	69:1k:101:3PE:H341	2.31	0.51
49:3E:206:LYS:O	49:3E:207:LYS:HD3	2.10	0.51
69:3J:105:3PE:H2D2	54:3Y:46:PRO:HG2	1.91	0.51
49:3R:180:THR:O	49:3R:181:LYS:C	2.53	0.51
91:4A:607:PGV:H302	75:4C:306:CDL:H402	1.92	0.51
58:4D:33:LEU:HD22	58:4D:37:GLN:HB3	1.92	0.51
1:1A:3:ILE:HG23	1:1A:4:MET:H	1.74	0.51
69:1B:204:3PE:H361	69:1B:205:3PE:H3B2	1.92	0.51
4:1D:20:TYR:N	14:1N:171:ASN:OD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:377:TYR:HB3	4:1D:390:LYS:HB3	1.92	0.51
6:1F:204:ARG:O	6:1F:205:LEU:C	2.51	0.51
6:1F:261:HIS:HD2	6:1F:337:MET:HA	1.75	0.51
7:1G:237:ASN:H	7:1G:259:ASN:ND2	2.08	0.51
7:1G:242:THR:HG21	7:1G:586:ALA:HB1	1.91	0.51
8:1H:131:GLY:HA2	8:1H:134:ARG:HG3	1.93	0.51
69:1L:712:3PE:H271	69:1L:204:3PE:H261	1.93	0.51
15:1O:101:TYR:O	15:1O:102:ALA:C	2.53	0.51
15:1O:261:MET:HA	15:1O:261:MET:HE2	1.91	0.51
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.44	0.51
20:1U:36:PHE:HD1	20:1U:40:LEU:HD12	1.75	0.51
46:3B:314:ALA:HA	49:3I:63:PRO:HD3	1.92	0.51
47:3C:287:LYS:HD2	69:3C:513:3PE:N	2.25	0.51
47:3C:302:ILE:HD11	69:3C:514:3PE:H3B1	1.93	0.51
49:3E:190:VAL:HG21	49:3E:250:ARG:HD3	1.92	0.51
52:3H:41:PRO:HG2	52:3H:102:LEU:CD2	2.41	0.51
49:3R:236:CYS:N	49:3R:242:HIS:HA	2.26	0.51
49:3R:250:ARG:C	49:3R:251:LYS:HD3	2.36	0.51
53:3W:11:TYR:HA	53:3W:15:PHE:HB2	1.92	0.51
54:3Y:41:ILE:HD12	69:3Y:105:3PE:C37	2.41	0.51
2:1B:175:ILE:HA	2:1B:178:ARG:HH11	1.75	0.51
69:1B:204:3PE:O21	69:1B:204:3PE:H242	2.10	0.51
4:1D:87:THR:HG23	4:1D:102:TYR:CD1	2.46	0.51
6:1F:405:CYS:SG	71:1F:502:SF4:S4	3.09	0.51
7:1G:114:CYS:O	7:1G:115:ASP:CB	2.57	0.51
9:1I:150:ASN:ND2	42:1q:127:TYR:O	2.43	0.51
12:1L:101:MET:HE1	12:1L:122:VAL:HG22	1.92	0.51
12:1L:467:ILE:HG21	69:1L:703:3PE:H371	1.93	0.51
12:1L:556:ILE:HG23	38:1m:79:PHE:CE1	2.46	0.51
13:1M:127:VAL:HB	13:1M:128:PRO:CD	2.41	0.51
24:1Y:27:ILE:CG2	69:1Y:208:3PE:H3D2	2.40	0.51
24:1Y:98:LEU:HD21	70:1Y:207:PC1:C27	2.40	0.51
70:1Y:207:PC1:H292	69:1Y:213:3PE:H2C2	1.92	0.51
33:1h:111:ARG:NH1	83:1h:201:AME:O	2.43	0.51
45:3A:362:ARG:HE	45:3A:396:GLU:CD	2.19	0.51
46:3B:277:HIS:CE1	46:3B:364:LEU:HD13	2.46	0.51
47:3C:310:SER:HB2	47:3C:370:SER:HB3	1.92	0.51
69:3C:513:3PE:H281	69:3C:513:3PE:H371	1.92	0.51
48:3D:284:GLU:OE2	48:3D:290:ARG:NH1	2.43	0.51
69:3E:302:3PE:H3A2	69:3E:302:3PE:H3E1	1.92	0.51
69:3G:101:3PE:H232	69:3G:102:3PE:O21	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:108:LYS:HE3	45:3N:112:LEU:HD11	1.92	0.51
46:3O:308:ASP:HB2	49:3V:55:LEU:HD13	1.92	0.51
47:3P:365:LEU:HD21	70:3T:102:PC1:H2I1	1.93	0.51
75:3P:513:CDL:H451	69:3P:520:3PE:C36	2.40	0.51
69:3P:514:3PE:H371	69:3Y:107:3PE:H351	1.92	0.51
75:3Y:106:CDL:HA62	69:3Y:107:3PE:C31	2.40	0.51
55:4A:84:PRO:HG3	55:4A:92:MET:HG2	1.93	0.51
56:4B:41:ILE:HB	56:4B:45:MET:HE2	1.92	0.51
4:1D:100:LEU:HD22	4:1D:195:ARG:HD3	1.91	0.51
11:1K:11:ALA:O	11:1K:14:ILE:HG13	2.11	0.51
13:1M:5:ILE:HG23	13:1M:104:LEU:HD11	1.93	0.51
13:1M:135:ARG:O	13:1M:135:ARG:HD3	2.11	0.51
14:1N:218:LEU:CD2	14:1N:240:ILE:HG23	2.41	0.51
15:1O:53:GLU:OE2	15:1O:126:ARG:HD2	2.10	0.51
15:1O:165:PRO:O	15:1O:248:TRP:NE1	2.40	0.51
17:1Q:28:GLU:H	17:1Q:28:GLU:CD	2.18	0.51
38:1m:101:TYR:CD1	69:1m:201:3PE:H281	2.46	0.51
45:3A:284:TYR:HD2	45:3A:290:MET:HE1	1.76	0.51
47:3C:132:VAL:HA	47:3C:139:SER:HB3	1.92	0.51
69:3C:513:3PE:H321	69:3C:513:3PE:O21	2.10	0.51
49:3E:242:HIS:CD2	49:3E:251:LYS:HD2	2.46	0.51
49:3E:257:ASN:ND2	49:3E:257:ASN:H	2.08	0.51
50:3F:31:TRP:CG	75:3F:201:CDL:H722	2.46	0.51
51:3G:55:VAL:O	51:3G:59:LEU:HG	2.11	0.51
69:3G:103:3PE:H112	69:3G:104:3PE:HN1	1.76	0.51
45:3N:139:GLN:HB2	49:3V:50:LEU:HD12	1.92	0.51
45:3N:145:MET:HA	45:3N:148:VAL:HG12	1.93	0.51
46:3O:293:SER:O	46:3O:297:GLN:HG2	2.11	0.51
69:3P:517:3PE:H3C1	69:3P:518:3PE:H3B1	1.92	0.51
48:3Q:180:SER:HG	52:3U:15:ASP:CG	2.17	0.51
49:3R:234:TYR:HD2	49:3R:243:TYR:HB3	1.75	0.51
56:4B:59:GLN:OE1	68:4N:14:SER:OG	2.20	0.51
57:4C:29:SER:O	57:4C:33:MET:HG2	2.10	0.51
57:4C:247:VAL:C	57:4C:249:TRP:N	2.66	0.51
91:4C:305:PGV:H311	91:4C:305:PGV:H172	1.91	0.51
62:4H:37:HIS:HB2	62:4H:85:ILE:HB	1.93	0.51
69:1A:203:3PE:H241	14:1N:2:ASN:HD22	1.76	0.51
7:1G:146:VAL:HG12	7:1G:200:ILE:CG1	2.41	0.51
7:1G:347:GLU:OE1	7:1G:495:ARG:NH2	2.44	0.51
22:1W:64:ARG:O	22:1W:68:MET:HG2	2.11	0.51
23:1X:23:VAL:HG21	26:1a:65:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1b:23:ALA:HA	69:1b:101:3PE:H2D2	1.93	0.51
75:1q:202:CDL:H171	75:1q:202:CDL:H621	1.92	0.51
46:3B:95:LYS:NZ	49:3I:69:GLY:HA3	2.25	0.51
47:3C:287:LYS:HG3	69:3C:513:3PE:H122	1.93	0.51
47:3C:296:ALA:HB2	69:3C:512:3PE:H3E1	1.92	0.51
46:3O:212:SER:O	46:3O:215:VAL:HG12	2.11	0.51
46:3O:248:ASN:OD1	46:3O:428:GLY:HA2	2.11	0.51
47:3P:286:ASN:HD21	69:3P:503:3PE:H242	1.75	0.51
75:3P:513:CDL:H352	75:3P:513:CDL:H161	1.93	0.51
75:3P:513:CDL:C39	69:3P:519:3PE:H2E1	2.41	0.51
48:3Q:231:LYS:HZ3	75:3T:101:CDL:H1O1	1.54	0.51
49:3R:150:SER:HB2	49:3R:170:ARG:HD3	1.92	0.51
70:3X:104:PC1:H261	70:3X:104:PC1:H222	1.93	0.51
54:3Y:41:ILE:HG13	69:3Y:105:3PE:H2B1	1.93	0.51
93:4B:303:PSC:H52	93:4B:303:PSC:H251	1.92	0.51
93:4B:303:PSC:H211	63:4I:17:LEU:CD2	2.39	0.51
69:1B:204:3PE:H352	69:1B:205:3PE:H3E1	1.92	0.51
6:1F:204:ARG:C	6:1F:205:LEU:O	2.54	0.51
8:1H:175:ILE:C	8:1H:177:THR:H	2.17	0.51
10:1J:99:MET:HG3	69:1J:201:3PE:H3I3	1.93	0.51
12:1L:604:TYR:CE2	14:1N:153:LEU:HD13	2.46	0.51
13:1M:41:LEU:O	13:1M:44:GLN:NE2	2.44	0.51
13:1M:133:ILE:HG12	13:1M:223:ALA:HB2	1.93	0.51
14:1N:298:TYR:O	14:1N:303:THR:OG1	2.21	0.51
16:1P:268:ARG:NH1	16:1P:268:ARG:O	2.43	0.51
28:1c:30:TYR:HE2	69:1d:203:3PE:C33	2.20	0.51
32:1g:36:ASN:HD21	32:1g:38:TYR:HB2	1.76	0.51
33:1h:35:PRO:HB2	70:1h:202:PC1:H2I1	1.93	0.51
69:3C:512:3PE:C31	69:3C:512:3PE:H231	2.40	0.51
69:3C:513:3PE:H121	69:3C:513:3PE:H11	1.93	0.51
69:3D:503:3PE:H2A1	69:3G:102:3PE:H382	1.92	0.51
49:3E:169:TRP:NE1	49:3E:273:VAL:HG12	2.26	0.51
49:3E:199:GLN:O	49:3E:248:ARG:HD3	2.10	0.51
49:3E:228:ALA:HA	49:3E:232:GLY:CA	2.40	0.51
51:3G:63:TRP:O	51:3G:66:GLN:HG3	2.11	0.51
45:3N:27:SER:OG	45:3N:205:HIS:HB2	2.11	0.51
54:3X:46:PRO:HG2	69:3X:101:3PE:C28	2.41	0.51
91:4A:609:PGV:H031	66:4L:24:MET:HE1	1.93	0.51
75:4C:306:CDL:HB61	75:4C:306:CDL:H542	1.93	0.51
68:4N:43:VAL:O	68:4N:53:PRO:HG3	2.11	0.51
2:1B:41:ARG:HH21	8:1H:57:THR:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:337:MET:HB3	6:1F:341:THR:HG21	1.93	0.50
8:1H:165:LEU:HD13	8:1H:241:LEU:HA	1.93	0.50
70:1H:402:PC1:H332	9:1I:27:TRP:CZ2	2.46	0.50
12:1L:467:ILE:HD12	69:1L:703:3PE:H322	1.93	0.50
14:1N:10:ILE:HG13	75:1N:402:CDL:H112	1.93	0.50
15:1O:104:ARG:C	15:1O:106:LEU:N	2.54	0.50
24:1Y:4:LEU:C	24:1Y:7:LYS:HG2	2.36	0.50
24:1Y:42:LEU:HD13	69:1Y:204:3PE:O32	2.11	0.50
29:1d:34:MET:CE	29:1d:37:LEU:HD12	2.42	0.50
69:1d:206:3PE:H3B2	69:1f:104:3PE:H2C1	1.93	0.50
46:3B:227:ARG:O	46:3B:228:GLY:C	2.54	0.50
46:3B:279:LEU:HD22	46:3B:295:LEU:HG	1.93	0.50
46:3B:308:ASP:HB2	49:3I:55:LEU:HB3	1.93	0.50
47:3C:77:TRP:CD2	48:3D:286:GLU:HG3	2.46	0.50
45:3N:445:ARG:NH2	69:3N:501:3PE:O12	2.44	0.50
46:3O:131:GLU:O	46:3O:132:PHE:C	2.54	0.50
48:3Q:77:ASP:OD1	48:3Q:77:ASP:N	2.42	0.50
49:3R:197:ASP:H	49:3R:248:ARG:NH2	2.09	0.50
49:3R:206:LYS:HG2	49:3R:263:TYR:OH	2.10	0.50
52:3U:50:THR:HG22	52:3U:51:GLU:H	1.76	0.50
69:3X:107:3PE:H121	69:4G:101:3PE:H12	1.93	0.50
55:4A:229:ILE:HD11	56:4B:175:ILE:HG21	1.93	0.50
91:4C:302:PGV:C6	91:4C:302:PGV:C01	2.89	0.50
2:1B:176:TRP:CH2	70:1B:202:PC1:H262	2.45	0.50
7:1G:613:TYR:HE2	7:1G:622:ARG:HG2	1.76	0.50
70:1H:402:PC1:H3E2	27:1b:24:ILE:HD11	1.92	0.50
9:1I:49:ASN:ND2	42:1q:30:ALA:O	2.39	0.50
9:1I:135:PRO:HD3	9:1I:165:ILE:HG22	1.92	0.50
14:1N:213:LEU:HB3	14:1N:217:MET:HE2	1.93	0.50
16:1P:84:VAL:HG23	16:1P:85:VAL:HG23	1.93	0.50
16:1P:133:SER:HA	16:1P:149:LYS:HE3	1.94	0.50
19:1S:20:ILE:HD11	19:1S:54:ILE:HG13	1.94	0.50
69:1Y:216:3PE:H242	69:1Y:216:3PE:H321	1.94	0.50
25:1Z:29:GLY:N	69:1Z:201:3PE:H111	2.24	0.50
70:1d:204:PC1:O14	70:1d:204:PC1:H132	2.10	0.50
69:1l:202:3PE:H2B2	69:1l:203:3PE:H361	1.93	0.50
43:1r:2:SER:N	43:1r:27:TYR:HH	2.09	0.50
45:3A:444:LEU:HD13	69:3A:502:3PE:H222	1.92	0.50
46:3B:126:VAL:HG23	46:3B:127:THR:HG23	1.92	0.50
69:3C:515:3PE:O13	70:3P:509:PC1:H112	2.11	0.50
45:3N:62:LEU:HD11	45:3N:127:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:68:LYS:HG2	45:3N:119:ASN:O	2.12	0.50
46:3O:45:SER:HB2	46:3O:116:ILE:HG12	1.92	0.50
69:3S:201:3PE:H392	70:3T:102:PC1:H262	1.93	0.50
52:3U:40:CYS:HA	52:3U:43:ARG:NH1	2.26	0.50
55:4A:72:PRO:O	55:4A:77:GLY:N	2.41	0.50
56:4B:65:TRP:HZ3	93:4B:303:PSC:H71	1.76	0.50
57:4C:54:MET:HE3	57:4C:58:TRP:CZ3	2.46	0.50
57:4C:204:HIS:CE1	57:4C:249:TRP:HB2	2.46	0.50
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.42	0.50
5:1E:104:THR:HG23	6:1F:349:ARG:HH21	1.76	0.50
11:1K:12:PHE:CE2	14:1N:72:MET:HG2	2.46	0.50
12:1L:217:LEU:HD12	12:1L:260:LEU:HD21	1.92	0.50
13:1M:10:MET:HE1	69:1f:104:3PE:C38	2.41	0.50
14:1N:129:LEU:HD13	75:1N:402:CDL:H541	1.93	0.50
15:1O:132:PHE:HZ	15:1O:210:PHE:HB2	1.75	0.50
38:1m:99:PHE:CG	69:1m:205:3PE:H3I2	2.46	0.50
75:1q:202:CDL:H191	75:1q:202:CDL:H372	1.93	0.50
43:1r:2:SER:HB2	43:1r:27:TYR:HE2	1.75	0.50
45:3A:349:ALA:H	45:3A:408:ARG:CG	2.23	0.50
47:3C:8:HIS:HB3	47:3C:11:MET:HB2	1.92	0.50
47:3C:314:SER:O	47:3C:318:ARG:HD3	2.11	0.50
49:3E:217:CYS:HB3	49:3E:221:GLY:CA	2.33	0.50
69:3G:110:3PE:H242	69:3G:110:3PE:H2B1	1.93	0.50
48:3Q:218:LEU:HD23	69:3R:305:3PE:C37	2.36	0.50
49:3R:153:GLU:HG3	49:3R:169:TRP:CG	2.46	0.50
49:3R:244:ASP:OD1	49:3R:248:ARG:HB2	2.10	0.50
49:3R:260:VAL:HG13	49:3R:263:TYR:CE2	2.46	0.50
50:3S:84:GLU:CD	50:3S:84:GLU:H	2.19	0.50
69:3W:103:3PE:C12	69:3W:103:3PE:H222	2.41	0.50
69:3W:103:3PE:H361	69:3W:103:3PE:H2A2	1.92	0.50
69:3X:101:3PE:H262	69:3X:101:3PE:H3D1	1.93	0.50
69:3X:105:3PE:H222	69:3X:105:3PE:O13	2.12	0.50
69:3X:108:3PE:H11	69:4G:104:3PE:H11	1.93	0.50
55:4A:377:PHE:O	55:4A:381:LEU:HB2	2.11	0.50
2:1B:69:MET:HB2	2:1B:74:VAL:HB	1.94	0.50
5:1E:37:ASN:C	44:1s:65:GLN:HE22	2.20	0.50
7:1G:584:LYS:HE2	17:1Q:36:ARG:HD2	1.92	0.50
12:1L:63:ILE:HD11	34:1i:85:LEU:HD22	1.92	0.50
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.11	0.50
13:1M:98:MET:HE1	69:1N:401:3PE:H3D1	1.94	0.50
29:1d:109:TYR:O	41:1p:159:LYS:NZ	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:25:TYR:CE1	69:1f:104:3PE:H221	2.42	0.50
48:3D:160:ASP:HB3	48:3D:169:PHE:CZ	2.46	0.50
48:3D:269:SER:HB2	52:3H:102:LEU:HD11	1.92	0.50
49:3E:219:HIS:C	49:3E:221:GLY:N	2.69	0.50
52:3H:82:GLU:N	52:3H:82:GLU:OE2	2.44	0.50
45:3N:19:LEU:HB2	45:3N:21:ASN:OD1	2.10	0.50
69:3P:511:3PE:C3C	69:3P:512:3PE:H3B1	2.42	0.50
49:3R:95:GLU:CD	49:3R:95:GLU:H	2.20	0.50
49:3R:199:GLN:CD	49:3R:257:ASN:HD21	2.19	0.50
54:3X:1:MET:HE3	69:3X:105:3PE:H242	1.93	0.50
69:3X:101:3PE:H32	69:3X:101:3PE:H351	1.93	0.50
69:3X:107:3PE:O14	69:4G:101:3PE:H322	2.12	0.50
69:3Y:102:3PE:H3B2	69:3Y:105:3PE:H3F1	1.93	0.50
55:4A:110:LEU:CA	91:4A:609:PGV:H181	2.42	0.50
58:4D:41:LYS:O	58:4D:45:LYS:NZ	2.44	0.50
1:1A:106:TRP:CD2	69:1A:201:3PE:H231	2.47	0.50
7:1G:378:LEU:HB3	7:1G:451:VAL:HG12	1.93	0.50
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	1.94	0.50
69:1L:709:3PE:C2D	75:1i:201:CDL:H182	2.41	0.50
13:1M:5:ILE:HG23	13:1M:104:LEU:CD1	2.40	0.50
24:1Y:75:ILE:CB	69:1Y:214:3PE:H282	2.42	0.50
25:1Z:140:PHE:CD1	26:1a:45:TRP:HB2	2.46	0.50
75:1g:201:CDL:HA4	33:1h:27:PHE:HE2	1.75	0.50
45:3A:368:HIS:C	45:3A:370:ASP:H	2.20	0.50
46:3B:226:MET:HG2	46:3B:227:ARG:N	2.27	0.50
48:3D:299:MET:HE1	69:3J:104:3PE:C3B	2.42	0.50
49:3E:93:ARG:NH2	51:3G:23:PHE:HA	2.26	0.50
49:3E:195:LEU:HD11	49:3E:248:ARG:HD2	1.93	0.50
49:3E:234:TYR:CD2	49:3E:247:GLY:HA2	2.46	0.50
49:3I:41:PRO:HB2	49:3I:44:ASP:HB3	1.93	0.50
46:3O:35:ILE:HD11	46:3O:220:ALA:CB	2.41	0.50
47:3P:65:SER:O	47:3P:69:ILE:HG13	2.12	0.50
47:3P:160:LEU:O	47:3P:164:ILE:HG13	2.12	0.50
47:3P:161:VAL:HG12	47:3P:165:TRP:CE2	2.47	0.50
75:3P:513:CDL:H431	69:3P:519:3PE:C2A	2.42	0.50
68:4N:44:CYS:HB2	68:4N:53:PRO:HG3	1.94	0.50
1:1A:33:LYS:HG2	8:1H:61:LEU:HD11	1.92	0.50
5:1E:48:LEU:HD21	5:1E:87:TYR:CZ	2.46	0.50
7:1G:522:LEU:HB3	7:1G:543:ILE:HG12	1.94	0.50
9:1I:74:GLU:HA	18:1R:40:ALA:HB1	1.92	0.50
13:1M:98:MET:HB2	13:1M:132:ILE:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:1N:402:CDL:C82	75:1d:205:CDL:H671	2.42	0.50
20:1U:83:LYS:HD3	20:1U:84:LYS:HD3	1.93	0.50
23:1X:43:MET:HG2	27:1b:52:TYR:CE2	2.46	0.50
23:1X:168:PHE:HE1	75:1d:202:CDL:H141	1.75	0.50
25:1Z:140:PHE:HB2	26:1a:45:TRP:CG	2.47	0.50
69:1f:103:3PE:H261	69:1f:104:3PE:H3G2	1.93	0.50
32:1g:88:TRP:CD1	41:1p:65:ARG:HB3	2.47	0.50
75:3A:501:CDL:H751	70:3J:106:PC1:H261	1.94	0.50
46:3B:286:LYS:HG2	46:3B:287:ARG:HG3	1.93	0.50
46:3B:291:ALA:C	46:3B:293:SER:N	2.69	0.50
47:3C:186:PRO:HA	47:3C:189:ILE:HD12	1.94	0.50
47:3C:281:LEU:HD12	47:3C:291:VAL:HA	1.92	0.50
69:3C:507:3PE:H282	69:3C:508:3PE:C26	2.35	0.50
69:3C:517:3PE:H371	69:3X:107:3PE:H2C1	1.93	0.50
48:3D:232:ARG:CD	49:3R:237:PRO:HB3	2.27	0.50
69:3J:104:3PE:H3I3	69:3J:105:3PE:H391	1.93	0.50
45:3N:242:ARG:NH2	45:3N:432:PRO:O	2.39	0.50
45:3N:381:ARG:HB3	45:3N:381:ARG:CZ	2.42	0.50
46:3O:395:PRO:O	46:3O:399:LEU:HG	2.11	0.50
47:3P:10:LEU:CD2	69:3P:512:3PE:H382	2.37	0.50
47:3P:318:ARG:O	47:3P:322:GLN:HG3	2.12	0.50
69:3P:504:3PE:C38	69:3Y:103:3PE:H271	2.42	0.50
48:3Q:237:TYR:HB2	50:3S:60:PHE:CG	2.47	0.50
49:3R:167:PHE:O	49:3R:173:PRO:HA	2.11	0.50
70:3R:303:PC1:H2I3	54:3X:32:LEU:HB2	1.94	0.50
54:3Y:41:ILE:HD11	69:3Y:105:3PE:H291	1.91	0.50
55:4A:80:ASN:OD1	55:4A:98:ASN:ND2	2.38	0.50
2:1B:32:LYS:NZ	69:1B:204:3PE:H281	2.26	0.50
7:1G:281:GLN:HG2	7:1G:592:LEU:HD12	1.92	0.50
7:1G:575:ASN:ND2	7:1G:577:GLU:OE2	2.45	0.50
12:1L:23:ASN:CB	69:1L:709:3PE:P	2.99	0.50
20:1T:28:GLU:N	20:1T:28:GLU:OE1	2.44	0.50
69:1d:201:3PE:C2H	75:1d:202:CDL:H461	2.42	0.50
75:1g:201:CDL:OB4	33:1h:23:LYS:CD	2.60	0.50
34:1i:107:ASP:OD1	34:1i:107:ASP:N	2.45	0.50
38:1m:24:ILE:O	45:3N:227:ALA:HA	2.11	0.50
41:1p:93:ARG:O	41:1p:97:VAL:HG23	2.10	0.50
45:3A:70:ARG:HD3	45:3A:78:GLU:OE1	2.12	0.50
75:3A:501:CDL:H582	75:3A:501:CDL:H622	1.92	0.50
46:3B:47:ILE:HD12	46:3B:216:LEU:HD21	1.94	0.50
47:3C:98:VAL:O	47:3C:102:LEU:HG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3C:515:3PE:H391	69:3C:515:3PE:C34	2.40	0.50
69:3C:515:3PE:H2C2	69:3C:516:3PE:H291	1.92	0.50
46:3O:35:ILE:CD1	46:3O:206:LEU:HB3	2.41	0.50
49:3R:206:LYS:CB	49:3R:265:PHE:HD2	2.24	0.50
49:3R:263:TYR:HB3	49:3R:273:VAL:HG22	1.94	0.50
56:4B:9:PHE:HB2	56:4B:21:LEU:HD21	1.94	0.50
91:4C:305:PGV:H101	75:4C:307:CDL:H802	1.92	0.50
68:4N:38:LEU:HB3	68:4N:39:PHE:CE2	2.47	0.50
70:1B:203:PC1:H281	75:1q:202:CDL:H181	1.94	0.50
4:1D:62:LEU:HD11	4:1D:78:PRO:HB3	1.94	0.50
5:1E:109:MET:O	5:1E:111:ARG:N	2.45	0.50
8:1H:173:TRP:HD1	70:1H:404:PC1:H142	1.76	0.50
9:1I:27:TRP:O	9:1I:30:LEU:HB2	2.12	0.50
13:1M:391:ILE:HG12	69:1M:502:3PE:H341	1.94	0.50
16:1P:132:ILE:HD11	16:1P:214:ILE:HD11	1.92	0.50
19:1S:64:LEU:HD11	19:1S:93:VAL:HG21	1.94	0.50
20:1T:6:LEU:HD23	20:1T:6:LEU:H	1.76	0.50
20:1T:28:GLU:H	20:1T:28:GLU:CD	2.19	0.50
20:1U:54:MET:HG3	20:1U:76:ILE:HG21	1.93	0.50
24:1Y:117:MET:HE3	69:1Y:205:3PE:H2B2	1.94	0.50
69:1f:102:3PE:H12	69:1f:102:3PE:H121	1.93	0.50
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.23	0.50
46:3B:227:ARG:C	46:3B:229:GLY:N	2.67	0.50
45:3N:302:LYS:HD2	45:3N:302:LYS:N	2.27	0.50
47:3P:272:TRP:HA	47:3P:275:LEU:HG	1.94	0.50
69:3P:512:3PE:H231	69:3X:105:3PE:C31	2.42	0.50
69:3P:512:3PE:H2H2	69:3P:512:3PE:H3B2	1.93	0.50
48:3Q:32:VAL:HG22	48:3Q:169:LEU:HD21	1.94	0.50
48:3Q:220:TYR:CE2	51:3T:26:PHE:HE2	2.29	0.50
69:3W:103:3PE:H372	69:3W:103:3PE:H2D1	1.93	0.50
55:4A:7:LEU:HD23	55:4A:103:TRP:CZ2	2.47	0.50
2:1B:176:TRP:CZ2	70:1B:202:PC1:H2A1	2.47	0.50
13:1M:23:ILE:HD11	13:1M:89:THR:HG23	1.94	0.50
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.94	0.50
75:1N:402:CDL:H631	69:1e:201:3PE:H3A2	1.94	0.50
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.44	0.50
29:1d:34:MET:HA	29:1d:34:MET:CE	2.34	0.50
30:1e:2:PHE:CE2	69:1e:201:3PE:H3H2	2.47	0.50
69:1h:204:3PE:H232	69:1h:204:3PE:P	2.52	0.50
37:1l:158:ILE:HG12	40:1o:99:LYS:HB3	1.94	0.50
47:3C:49:LEU:O	47:3C:53:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3D:503:3PE:C22	69:3G:101:3PE:H222	2.37	0.50
49:3E:187:GLU:HA	49:3E:190:VAL:HG23	1.94	0.50
49:3E:219:HIS:HB2	72:3E:301:FES:S1	2.52	0.50
49:3E:263:TYR:CB	49:3E:273:VAL:HG22	2.40	0.50
50:3F:86:ILE:HD12	50:3F:92:TRP:HZ2	1.77	0.50
69:3G:110:3PE:H282	69:3G:110:3PE:C24	2.39	0.50
53:3J:35:ALA:HB1	69:3J:104:3PE:H2E2	1.94	0.50
69:3N:501:3PE:H382	75:3N:502:CDL:C16	2.40	0.50
91:4C:303:PGV:C20	68:4N:36:LEU:HB3	2.39	0.50
5:1E:106:THR:HA	5:1E:109:MET:HB3	1.94	0.49
12:1L:562:LEU:CD2	69:1L:705:3PE:H3B1	2.41	0.49
14:1N:10:ILE:HG21	75:1N:402:CDL:H121	1.94	0.49
15:1O:136:GLU:O	15:1O:140:ARG:HG2	2.12	0.49
23:1X:34:GLN:HE22	23:1X:116:TRP:CD1	2.30	0.49
23:1X:82:THR:HA	23:1X:85:TRP:NE1	2.26	0.49
24:1Y:76:SER:CA	69:1Y:214:3PE:H221	2.39	0.49
75:1Y:217:CDL:H112	75:1Y:217:CDL:H152	1.93	0.49
69:1f:102:3PE:H281	69:1g:202:3PE:C3D	2.38	0.49
40:1o:25:PRO:HD2	40:1o:28:TYR:HD2	1.77	0.49
45:3A:363:ASN:HD22	46:3B:93:GLY:HA3	1.76	0.49
47:3C:318:ARG:O	47:3C:322:GLN:HG3	2.12	0.49
51:3G:36:ILE:HB	51:3G:37:PRO:HD3	1.94	0.49
52:3H:68:ARG:O	52:3H:72:ARG:HG3	2.12	0.49
69:3P:514:3PE:H3C2	69:3P:514:3PE:H291	1.94	0.49
49:3R:212:ILE:HD13	49:3R:265:PHE:CE1	2.47	0.49
51:3T:26:PHE:CE2	69:3T:103:3PE:H362	2.47	0.49
69:3X:108:3PE:H3F2	69:3X:108:3PE:H2I2	1.93	0.49
75:3Y:106:CDL:H192	75:3Y:106:CDL:H251	1.94	0.49
55:4A:428:GLN:HA	55:4A:431:LEU:HD12	1.94	0.49
58:4D:124:LEU:O	58:4D:140:TYR:OH	2.18	0.49
1:1A:6:THR:HA	8:1H:6:ILE:HD13	1.94	0.49
9:1I:52:PHE:CZ	42:1q:30:ALA:HA	2.47	0.49
11:1K:14:ILE:C	11:1K:14:ILE:HD12	2.37	0.49
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.93	0.49
12:1L:296:ASN:OD1	39:1n:77:GLN:NE2	2.45	0.49
12:1L:467:ILE:HG22	69:1o:201:3PE:H2I1	1.93	0.49
69:1L:711:3PE:C23	69:1M:502:3PE:H231	2.42	0.49
13:1M:1:FME:HE3	13:1M:111:THR:HG21	1.94	0.49
23:1X:17:VAL:HG11	25:1Z:74:LEU:HD11	1.94	0.49
24:1Y:28:GLY:HA2	69:1Y:208:3PE:H382	1.94	0.49
69:1d:206:3PE:H382	69:1f:104:3PE:H292	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:92:PHE:CG	69:1m:203:3PE:H271	2.35	0.49
38:1m:101:TYR:CZ	69:1m:201:3PE:H271	2.46	0.49
47:3C:133:LEU:N	47:3C:134:PRO:HD2	2.27	0.49
47:3C:137:GLN:HB2	47:3C:254:ASP:O	2.11	0.49
47:3C:284:ILE:HD13	69:3C:512:3PE:C26	2.43	0.49
46:3O:45:SER:N	46:3O:111:CYS:O	2.34	0.49
46:3O:307:PHE:O	49:3V:52:ARG:HG3	2.12	0.49
47:3P:6:LYS:O	47:3P:12:LYS:HE3	2.12	0.49
48:3Q:134:TYR:CD2	48:3Q:162:PRO:HG3	2.47	0.49
69:3Y:102:3PE:H3B2	69:3Y:105:3PE:C3E	2.42	0.49
69:3Y:102:3PE:H291	69:3Y:105:3PE:H121	1.94	0.49
55:4A:279:SER:HB3	68:4N:22:ILE:HG12	1.94	0.49
55:4A:383:MET:HE2	55:4A:425:PHE:HD2	1.76	0.49
56:4B:29:MET:SD	63:4I:36:LYS:HB2	2.53	0.49
56:4B:70:ALA:O	56:4B:74:ILE:HG23	2.12	0.49
93:4B:303:PSC:H032	93:4B:303:PSC:H073	1.92	0.49
57:4C:220:LEU:HD21	75:4C:307:CDL:H232	1.93	0.49
58:4D:141:ASP:O	58:4D:143:ASN:N	2.44	0.49
61:4G:78:LEU:N	61:4G:81:GLY:O	2.43	0.49
2:1B:176:TRP:HA	2:1B:179:ARG:HD2	1.94	0.49
8:1H:286:MET:HE2	8:1H:286:MET:HA	1.95	0.49
12:1L:146:GLY:HA2	75:1L:704:CDL:H762	1.94	0.49
12:1L:253:VAL:HB	12:1L:310:LEU:HD11	1.94	0.49
12:1L:556:ILE:CD1	38:1m:79:PHE:HB2	2.42	0.49
13:1M:135:ARG:HG3	69:1N:401:3PE:H362	1.94	0.49
16:1P:194:ILE:HD12	16:1P:288:HIS:CD2	2.41	0.49
69:1Y:209:3PE:H362	69:1Y:213:3PE:C25	2.41	0.49
29:1d:9:VAL:O	70:1d:204:PC1:H222	2.13	0.49
35:1j:34:PHE:HE2	69:1k:101:3PE:H3D1	1.78	0.49
38:1m:92:PHE:CB	69:1m:203:3PE:H291	2.42	0.49
40:1o:24:PHE:HD2	40:1o:107:LEU:HD13	1.77	0.49
47:3C:116:GLY:C	85:3C:502:HEM:HBC2	2.37	0.49
47:3C:368:ILE:HG22	69:3C:507:3PE:H271	1.94	0.49
49:3E:191:GLU:HB3	49:3E:194:GLN:HG2	1.93	0.49
53:3J:11:TYR:HA	53:3J:15:PHE:HB2	1.93	0.49
46:3O:275:LEU:HB2	46:3O:410:VAL:HG13	1.93	0.49
46:3O:366:ALA:HB1	46:3O:370:MET:HE3	1.94	0.49
75:3P:513:CDL:H511	51:3T:40:ARG:CZ	2.43	0.49
48:3Q:27:ARG:NE	48:3Q:55:CYS:O	2.45	0.49
49:3R:236:CYS:HB3	49:3R:241:SER:N	2.27	0.49
54:3X:1:MET:HG3	69:3X:105:3PE:H241	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:4C:161:GLN:HA	91:4C:302:PGV:H101	1.94	0.49
7:1G:174:THR:OG1	7:1G:181:MET:HG2	2.11	0.49
75:1L:704:CDL:H602	13:1M:371:PRO:HD2	1.93	0.49
13:1M:41:LEU:HD13	13:1M:66:LEU:HD13	1.94	0.49
15:1O:298:GLU:O	15:1O:299:LEU:C	2.51	0.49
20:1T:76:ILE:O	20:1T:80:ILE:HG12	2.12	0.49
24:1Y:87:LEU:CD1	69:1Y:212:3PE:C33	2.78	0.49
70:1Y:206:PC1:C12	38:1m:81:PRO:HD3	2.41	0.49
69:1Y:213:3PE:H3A2	38:1m:94:ILE:HD12	1.94	0.49
32:1g:63:PHE:O	32:1g:67:SER:HB2	2.12	0.49
45:3A:445:ARG:NH1	75:3A:501:CDL:OB3	2.45	0.49
69:3C:506:3PE:H3C1	69:3C:506:3PE:H381	1.93	0.49
69:3G:101:3PE:O13	69:3G:108:3PE:N	2.41	0.49
49:3I:36:ALA:HB3	49:3I:73:PRO:HG2	1.94	0.49
48:3Q:160:MET:HB2	86:3Q:501:HEC:C1D	2.42	0.49
69:3Y:101:3PE:H392	69:3Y:102:3PE:H3H1	1.94	0.49
56:4B:23:PHE:CZ	56:4B:80:SER:HB2	2.48	0.49
57:4C:160:ILE:HG23	57:4C:219:LEU:HD11	1.93	0.49
1:1A:54:LYS:HB3	1:1A:113:TRP:CE3	2.47	0.49
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.12	0.49
16:1P:216:ASN:ND2	16:1P:303:LEU:O	2.45	0.49
27:1b:30:ILE:HG22	27:1b:34:LEU:HD11	1.94	0.49
28:1c:26:PHE:CD2	75:1d:205:CDL:H821	2.47	0.49
75:1g:201:CDL:C67	69:1h:204:3PE:H3I3	2.43	0.49
37:1l:74:GLY:HA3	38:1m:42:LEU:HD22	1.94	0.49
38:1m:19:PRO:HA	38:1m:22:TYR:CE2	2.48	0.49
69:1m:202:3PE:H2D2	69:1m:202:3PE:C3B	2.42	0.49
69:1m:202:3PE:H321	51:3T:31:THR:HA	1.93	0.49
45:3A:445:ARG:NH2	75:3A:501:CDL:HB21	2.27	0.49
47:3C:284:ILE:HG21	69:3C:512:3PE:H351	1.93	0.49
49:3E:189:ALA:O	49:3E:190:VAL:C	2.56	0.49
69:3G:105:3PE:N	69:3G:105:3PE:H11	2.28	0.49
45:3N:373:THR:HB	45:3N:374:PRO:HD3	1.94	0.49
69:3N:503:3PE:O31	69:3N:503:3PE:H342	2.12	0.49
70:3P:509:PC1:H342	69:3P:514:3PE:C3A	2.40	0.49
69:3Q:502:3PE:O14	69:3Q:502:3PE:H121	2.13	0.49
49:3R:246:SER:O	49:3R:248:ARG:N	2.46	0.49
69:3W:103:3PE:C27	91:4C:302:PGV:H22	2.42	0.49
54:3X:18:ILE:CG2	69:3X:106:3PE:H232	2.43	0.49
55:4A:52:GLN:O	55:4A:56:VAL:HG13	2.13	0.49
55:4A:240:HIS:O	55:4A:243:VAL:HB	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:403:TYR:CZ	55:4A:479:LYS:HG2	2.48	0.49
1:1A:51:PHE:O	1:1A:52:SER:HB3	2.13	0.49
2:1B:176:TRP:CD2	70:1B:202:PC1:H231	2.35	0.49
10:1J:28:TYR:HE2	10:1J:82:VAL:HG23	1.78	0.49
11:1K:26:LEU:O	11:1K:30:LEU:HG	2.12	0.49
14:1N:301:SER:C	69:1N:401:3PE:H342	2.33	0.49
17:1Q:85:THR:HG23	21:1V:115:ILE:HD11	1.94	0.49
75:1Y:217:CDL:OB8	75:1Y:217:CDL:H731	2.12	0.49
25:1Z:72:MET:HE3	27:1b:52:TYR:HD1	1.77	0.49
29:1d:36:PHE:HA	69:1d:206:3PE:H2C2	1.93	0.49
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.94	0.49
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.94	0.49
75:3A:501:CDL:H772	69:3A:502:3PE:C2E	2.42	0.49
46:3B:253:VAL:HA	46:3B:427:SER:O	2.12	0.49
47:3C:199:PHE:HE1	47:3P:9:PRO:HG2	1.78	0.49
47:3C:379:TRP:CZ3	50:3F:49:ILE:HD12	2.48	0.49
69:3C:509:3PE:O12	69:3X:107:3PE:H32	2.12	0.49
69:3C:513:3PE:H322	69:3C:517:3PE:C3	2.42	0.49
49:3E:159:ILE:CG1	49:3E:165:MET:HB2	2.43	0.49
49:3E:206:LYS:HZ1	49:3E:264:GLU:HA	1.77	0.49
49:3E:237:PRO:HB2	48:3Q:144:ARG:HD3	1.94	0.49
45:3N:141:ASN:HA	49:3V:47:ARG:NH2	2.20	0.49
45:3N:161:THR:HG22	49:3R:99:SER:HB2	1.94	0.49
47:3P:248:ASP:O	69:3P:520:3PE:H111	2.13	0.49
75:3P:513:CDL:H661	51:3T:38:LEU:HD21	1.95	0.49
69:3P:519:3PE:H2B2	69:3P:520:3PE:H371	1.94	0.49
49:3R:150:SER:O	49:3R:152:ILE:N	2.45	0.49
50:3S:32:MET:HB3	50:3S:86:ASP:OD1	2.12	0.49
54:3X:22:SER:HB2	69:3X:106:3PE:H2B2	1.94	0.49
75:3X:103:CDL:C22	69:3X:105:3PE:H3H2	2.42	0.49
69:3X:107:3PE:H372	69:3X:107:3PE:H331	1.95	0.49
55:4A:33:LEU:HB3	55:4A:61:HIS:HB2	1.94	0.49
55:4A:37:ILE:HD11	55:4A:58:VAL:HA	1.95	0.49
55:4A:128:VAL:O	55:4A:128:VAL:HG12	2.13	0.49
56:4B:94:ALA:HB3	56:4B:148:MET:HE3	1.95	0.49
56:4B:156:SER:OG	56:4B:159:VAL:O	2.28	0.49
57:4C:163:LEU:HB3	57:4C:219:LEU:HD13	1.94	0.49
58:4D:78:TRP:O	58:4D:82:VAL:HG23	2.13	0.49
1:1A:48:ARG:H	8:1H:126:LYS:HZ1	1.60	0.49
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.46	0.49
13:1M:201:MET:O	13:1M:205:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:337:VAL:HG23	13:1M:339:SER:H	1.78	0.49
14:1N:20:VAL:HG13	14:1N:29:ILE:HG23	1.94	0.49
14:1N:329:MET:CE	75:1N:402:CDL:H781	2.40	0.49
24:1Y:38:TYR:CD2	69:1Y:204:3PE:H372	2.46	0.49
69:1Y:209:3PE:H2B1	69:1m:202:3PE:H382	1.93	0.49
32:1g:75:THR:HG22	75:1i:201:CDL:H141	1.95	0.49
69:1k:101:3PE:C12	69:1o:201:3PE:H222	2.42	0.49
37:1l:41:GLY:O	38:1m:79:PHE:HD1	1.95	0.49
41:1p:116:GLU:HG3	41:1p:123:ASN:HB2	1.94	0.49
42:1q:68:MET:SD	42:1q:81:MET:HG2	2.53	0.49
46:3B:365:LYS:HG2	46:3B:399:LEU:HD22	1.94	0.49
47:3C:299:LEU:HD13	69:3C:512:3PE:H3I1	1.94	0.49
69:3C:503:3PE:O13	69:3C:505:3PE:H222	2.13	0.49
49:3E:156:LEU:C	49:3E:158:ASP:H	2.19	0.49
49:3E:263:TYR:CD1	49:3E:263:TYR:C	2.90	0.49
49:3E:273:VAL:CG2	49:3E:274:GLY:H	2.15	0.49
51:3G:35:GLY:O	51:3G:39:VAL:HG23	2.13	0.49
69:3J:103:3PE:H232	69:3J:103:3PE:H321	1.95	0.49
70:3J:106:PC1:H2F1	69:3P:507:3PE:H3I1	1.95	0.49
69:3P:511:3PE:C21	69:3P:511:3PE:H252	2.43	0.49
69:3P:515:3PE:H3A1	69:3P:516:3PE:H2I2	1.95	0.49
55:4A:23:GLY:HA3	55:4A:73:ILE:HG13	1.95	0.49
55:4A:73:ILE:HD13	88:4A:601:HEA:H242	1.94	0.49
91:4A:609:PGV:H32	91:4A:609:PGV:C21	2.34	0.49
58:4D:26:ASP:OD1	58:4D:26:ASP:N	2.33	0.49
69:1B:204:3PE:H332	69:1B:204:3PE:H372	1.95	0.49
3:1C:71:GLN:HG3	3:1C:101:PHE:CE2	2.48	0.49
10:1J:119:PHE:CE1	11:1K:1:FME:HE2	2.47	0.49
13:1M:190:TRP:O	13:1M:194:PHE:HD2	1.96	0.49
75:1N:402:CDL:H741	69:1e:201:3PE:H341	1.94	0.49
16:1P:48:PRO:HB3	16:1P:84:VAL:HG11	1.93	0.49
26:1a:4:GLU:O	26:1a:7:PRO:HD2	2.13	0.49
40:1o:14:LYS:HD3	40:1o:112:LYS:HG3	1.94	0.49
45:3A:354:VAL:HG21	45:3A:404:ALA:HA	1.95	0.49
46:3B:243:GLU:HB2	46:3B:436:VAL:CG2	2.43	0.49
47:3C:168:PHE:HZ	49:3R:151:LYS:HD3	1.77	0.49
49:3E:206:LYS:HD2	49:3E:263:TYR:CE1	2.47	0.49
69:3G:103:3PE:H372	69:3G:103:3PE:H272	1.95	0.49
46:3O:71:LEU:HD12	49:3V:68:VAL:HG11	1.95	0.49
47:3P:333:ILE:HD11	69:3P:508:3PE:H3A2	1.95	0.49
69:3P:503:3PE:C24	69:3P:503:3PE:H11	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:213:LEU:CD2	49:3R:258:LEU:HB2	2.42	0.49
69:3W:101:3PE:H262	69:3W:101:3PE:H372	1.94	0.49
55:4A:28:MET:HE2	67:4M:26:PHE:CE2	2.47	0.49
59:4E:69:GLU:HG2	59:4E:101:PRO:HG3	1.94	0.49
1:1A:13:LEU:HD13	8:1H:10:ILE:HG21	1.95	0.49
2:1B:60:MET:HA	2:1B:76:PHE:HZ	1.77	0.49
10:1J:14:VAL:O	10:1J:18:VAL:HG23	2.13	0.49
12:1L:603:ASN:HB3	69:1L:706:3PE:H121	1.94	0.49
75:1N:402:CDL:H352	75:1N:402:CDL:H382	1.55	0.49
17:1Q:89:LYS:NZ	17:1Q:107:GLU:OE1	2.46	0.49
20:1U:72:CYS:N	20:1U:75:GLU:OE1	2.44	0.49
22:1W:65:GLU:HG3	22:1W:66:MET:HE2	1.95	0.49
24:1Y:4:LEU:O	24:1Y:7:LYS:HG2	2.13	0.49
24:1Y:21:ALA:O	24:1Y:25:THR:OG1	2.31	0.49
24:1Y:72:THR:O	24:1Y:76:SER:OG	2.24	0.49
29:1d:29:PRO:HG2	75:1d:202:CDL:HA31	1.95	0.49
29:1d:32:VAL:HG13	69:1f:104:3PE:H2B2	1.93	0.49
31:1f:20:PHE:CD2	69:1f:103:3PE:H3C1	2.48	0.49
75:1g:201:CDL:H432	70:1h:202:PC1:H2G2	1.94	0.49
34:1i:57:LYS:HA	34:1i:60:ILE:HG22	1.95	0.49
37:1l:62:TYR:HD1	37:1l:63:ASP:N	2.10	0.49
75:1q:202:CDL:H622	75:1q:202:CDL:H872	1.95	0.49
45:3A:332:ASP:OD1	45:3A:432:PRO:HG3	2.13	0.49
46:3B:341:TYR:CE2	46:3B:345:LYS:HE2	2.48	0.49
69:3C:506:3PE:H342	69:3C:506:3PE:C29	2.43	0.49
69:3C:509:3PE:C28	69:3X:107:3PE:H3D1	2.43	0.49
49:3I:36:ALA:C	49:3I:38:SER:N	2.71	0.49
75:3N:502:CDL:H791	70:3R:303:PC1:H2F1	1.95	0.49
75:3N:502:CDL:H862	54:3X:25:GLY:HA2	1.94	0.49
46:3O:277:HIS:NE2	46:3O:364:LEU:HD13	2.27	0.49
52:3U:43:ARG:HD2	52:3U:52:GLU:OE1	2.13	0.49
53:3W:54:LYS:HA	53:3W:57:LYS:HD2	1.94	0.49
55:4A:38:ARG:HD3	55:4A:455:SER:HA	1.95	0.49
64:4J:41:GLY:HA3	91:4J:101:PGV:H292	1.95	0.49
70:1A:202:PC1:H221	70:1A:202:PC1:H321	1.94	0.49
8:1H:197:PRO:HB2	8:1H:280:PHE:HD2	1.77	0.49
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.31	0.49
12:1L:209:PRO:HG2	12:1L:213:LEU:HD11	1.95	0.49
69:1L:711:3PE:H2A2	69:1L:204:3PE:H3A2	1.94	0.49
15:1O:38:LEU:O	15:1O:39:ALA:C	2.54	0.49
15:1O:149:VAL:O	15:1O:153:ASN:ND2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:59:ARG:HB3	75:1g:201:CDL:C16	2.38	0.49
38:1m:92:PHE:HA	69:1m:203:3PE:H291	1.94	0.49
41:1p:78:GLU:HG2	41:1p:79:LYS:HG2	1.93	0.49
42:1q:3:LEU:HD23	75:1q:201:CDL:HB4	1.93	0.49
45:3A:112:LEU:O	45:3A:116:ILE:HG13	2.12	0.49
46:3B:181:TYR:CE2	46:3B:182:ARG:HG2	2.48	0.49
69:3C:503:3PE:H232	69:3C:503:3PE:O32	2.13	0.49
75:3F:201:CDL:CB7	75:3F:201:CDL:H531	2.43	0.49
48:3Q:135:CYS:SG	48:3Q:151:PRO:HG3	2.52	0.49
48:3Q:176:PRO:HB3	52:3U:13:LEU:HD11	1.95	0.49
49:3R:113:PHE:CE1	69:3R:305:3PE:H291	2.48	0.49
49:3R:236:CYS:SG	49:3R:239:HIS:HB2	2.53	0.49
69:3X:101:3PE:H352	69:3X:101:3PE:C31	2.43	0.49
69:3X:108:3PE:H11	69:3X:108:3PE:O22	2.13	0.49
69:3X:108:3PE:C3F	69:3X:108:3PE:H2G1	2.43	0.49
55:4A:110:LEU:N	91:4A:609:PGV:H181	2.27	0.49
57:4C:58:TRP:CD1	57:4C:61:ILE:HD12	2.47	0.49
62:4H:71:ALA:O	62:4H:75:ARG:HG3	2.13	0.49
3:1C:41:GLN:HG2	3:1C:51:PHE:HE2	1.78	0.48
6:1F:262:VAL:HG11	6:1F:284:ALA:HB1	1.95	0.48
7:1G:180:ASP:OD1	7:1G:180:ASP:N	2.46	0.48
10:1J:95:SER:O	10:1J:98:MET:HG2	2.12	0.48
12:1L:136:ASN:OD1	12:1L:139:GLN:HB2	2.13	0.48
12:1L:505:ASN:O	12:1L:508:THR:OG1	2.21	0.48
29:1d:31:LEU:O	29:1d:34:MET:HB2	2.13	0.48
37:1l:16:THR:HG23	37:1l:19:GLU:HG2	1.95	0.48
46:3B:227:ARG:HD3	46:3B:231:GLY:N	2.25	0.48
49:3E:190:VAL:CG1	49:3E:195:LEU:HD21	2.43	0.48
49:3E:229:GLY:HA3	49:3E:235:TYR:HB3	1.95	0.48
50:3F:27:GLY:O	50:3F:28:ILE:C	2.55	0.48
47:3P:108:MET:HA	47:3P:108:MET:CE	2.41	0.48
49:3R:161:GLU:CG	49:3R:180:THR:HB	2.43	0.48
75:3X:103:CDL:HB4	75:3X:103:CDL:OA7	2.12	0.48
55:4A:32:ALA:HB3	66:4L:36:PRO:HG2	1.95	0.48
55:4A:69:MET:HE1	55:4A:386:VAL:HG22	1.95	0.48
64:4J:15:ASP:OD1	64:4J:15:ASP:N	2.44	0.48
4:1D:47:LEU:O	4:1D:67:GLU:HA	2.12	0.48
12:1L:591:PHE:CZ	14:1N:111:PHE:HA	2.48	0.48
14:1N:129:LEU:CD1	75:1N:402:CDL:H541	2.43	0.48
16:1P:179:LEU:HA	16:1P:182:PHE:HB2	1.94	0.48
21:1V:4:LEU:HD23	21:1V:4:LEU:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:46:THR:HG22	22:1W:52:LEU:HD11	1.94	0.48
22:1W:47:VAL:HA	22:1W:52:LEU:HD12	1.93	0.48
24:1Y:62:SER:O	69:1Y:208:3PE:H381	2.11	0.48
69:1f:103:3PE:H342	70:1h:203:PC1:H222	1.94	0.48
75:1q:202:CDL:OB8	75:1q:202:CDL:H531	2.13	0.48
69:3N:503:3PE:H2I2	70:3X:104:PC1:H3I3	1.94	0.48
47:3P:341:GLN:HE22	69:3P:519:3PE:H121	1.78	0.48
69:3R:305:3PE:H3B1	69:3R:305:3PE:C3F	2.41	0.48
56:4B:221:LYS:HE3	56:4B:221:LYS:HA	1.93	0.48
75:4B:302:CDL:H202	75:4B:302:CDL:H172	1.68	0.48
58:4D:76:ASN:HD22	58:4D:79:LYS:NZ	2.11	0.48
69:1A:201:3PE:H321	69:1b:101:3PE:C1	2.43	0.48
4:1D:270:ARG:HG3	4:1D:368:GLU:HB3	1.95	0.48
12:1L:24:SER:CA	69:1L:710:3PE:P	2.94	0.48
15:1O:3:TYR:HE1	15:1O:12:GLU:HB3	1.77	0.48
15:1O:137:ALA:O	15:1O:139:TYR:N	2.46	0.48
22:1W:23:ARG:CZ	22:1W:23:ARG:HB3	2.42	0.48
24:1Y:100:LEU:HD21	69:1Y:205:3PE:O21	2.13	0.48
69:1d:206:3PE:H382	69:1f:104:3PE:H2A2	1.92	0.48
30:1e:31:ARG:NH2	30:1e:66:LEU:O	2.45	0.48
39:1n:166:TRP:O	39:1n:170:VAL:HG12	2.14	0.48
42:1q:20:LEU:HD11	75:1q:202:CDL:H412	1.95	0.48
46:3B:153:GLN:HE22	49:3I:42:VAL:HA	1.78	0.48
48:3D:232:ARG:O	48:3D:235:LEU:HB2	2.14	0.48
48:3D:272:ALA:O	48:3D:275:VAL:HG12	2.13	0.48
45:3N:188:GLN:OE1	45:3N:229:PRO:HD3	2.13	0.48
45:3N:445:ARG:NE	75:3N:502:CDL:OB3	2.42	0.48
47:3P:92:ILE:HG13	47:3P:272:TRP:CH2	2.49	0.48
47:3P:92:ILE:HG13	47:3P:272:TRP:HH2	1.79	0.48
47:3P:126:THR:HG21	47:3P:186:PRO:HG3	1.95	0.48
69:3P:508:3PE:H3I1	75:3P:513:CDL:H442	1.94	0.48
49:3R:267:SER:O	49:3R:271:VAL:HG13	2.13	0.48
69:3S:201:3PE:H381	70:3T:102:PC1:H271	1.95	0.48
69:3Y:102:3PE:H3B2	69:3Y:105:3PE:C3F	2.42	0.48
56:4B:35:SER:HB2	75:4B:302:CDL:C40	2.42	0.48
57:4C:224:LYS:HZ1	75:4C:307:CDL:HB4	1.78	0.48
91:4G:102:PGV:H251	91:4G:102:PGV:C13	2.39	0.48
1:1A:23:TRP:C	70:1A:202:PC1:H121	2.38	0.48
7:1G:655:GLN:OE1	7:1G:655:GLN:N	2.44	0.48
12:1L:553:LEU:HD21	38:1m:93:GLY:HA2	1.96	0.48
69:1L:705:3PE:C3E	82:1Y:203:PGT:H482	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:50:HIS:NE2	15:1O:125:GLU:OE2	2.44	0.48
24:1Y:27:ILE:HD12	69:1Y:208:3PE:C3I	2.43	0.48
29:1d:8:ARG:HH22	29:1d:82:MET:HE1	1.79	0.48
75:1g:201:CDL:H652	33:1h:35:PRO:CG	2.41	0.48
41:1p:130:GLN:O	41:1p:134:VAL:HG23	2.13	0.48
46:3B:215:VAL:O	46:3B:219:VAL:HG23	2.13	0.48
46:3B:247:GLN:HA	46:3B:428:GLY:O	2.13	0.48
69:3C:509:3PE:H3H1	75:3N:502:CDL:H851	1.95	0.48
69:3C:510:3PE:O11	69:3C:510:3PE:C21	2.55	0.48
50:3F:24:TRP:O	50:3F:28:ILE:HG13	2.13	0.48
50:3F:117:GLU:CD	54:3X:4:ARG:HD3	2.38	0.48
45:3N:258:GLU:HB3	49:3R:104:LYS:HE2	1.95	0.48
45:3N:268:VAL:O	45:3N:272:VAL:HG23	2.13	0.48
69:3P:511:3PE:H331	69:3P:512:3PE:H322	1.95	0.48
48:3Q:105:ASN:HD21	48:3Q:110:PRO:CD	2.27	0.48
49:3R:151:LYS:HG3	49:3R:152:ILE:HG12	1.95	0.48
55:4A:51:ASP:O	55:4A:55:ASN:ND2	2.38	0.48
62:4H:49:ASP:OD1	62:4H:49:ASP:O	2.32	0.48
1:1A:25:PRO:HB2	8:1H:60:PRO:HD3	1.95	0.48
2:1B:62:MET:HE3	2:1B:69:MET:SD	2.54	0.48
69:1B:204:3PE:H372	69:1B:204:3PE:C33	2.42	0.48
5:1E:148:CYS:C	5:1E:150:ASN:N	2.70	0.48
6:1F:28:ARG:HB3	44:1s:35:ASN:HA	1.96	0.48
6:1F:297:VAL:HA	6:1F:336:VAL:HA	1.95	0.48
11:1K:1:FME:HG2	11:1K:2:PRO:HD2	1.95	0.48
20:1U:18:VAL:O	20:1U:21:LEU:HB2	2.13	0.48
69:1Y:201:3PE:H362	69:3P:508:3PE:H3E2	1.96	0.48
29:1d:86:ARG:O	29:1d:90:MET:HB2	2.14	0.48
30:1e:32:CYS:SG	30:1e:66:LEU:HD23	2.54	0.48
35:1j:38:TRP:HE1	69:1k:101:3PE:C38	2.08	0.48
69:3C:503:3PE:O32	69:3C:503:3PE:H342	2.12	0.48
69:3C:506:3PE:H241	69:3C:506:3PE:O21	2.14	0.48
49:3E:219:HIS:O	49:3E:221:GLY:N	2.47	0.48
50:3F:107:LYS:HE2	50:3F:111:ARG:HH12	1.77	0.48
53:3J:15:PHE:O	70:3J:106:PC1:H151	2.13	0.48
45:3N:45:SER:HB3	45:3N:167:VAL:HA	1.94	0.48
46:3O:116:ILE:HG22	46:3O:120:MET:HE2	1.95	0.48
49:3R:181:LYS:O	49:3R:183:GLU:N	2.46	0.48
54:3X:18:ILE:HG22	69:3X:106:3PE:H232	1.94	0.48
54:3X:38:TRP:HA	70:3X:104:PC1:H32	1.95	0.48
65:4K:19:ALA:O	65:4K:23:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:1:FME:HG3	25:1Z:142:TRP:CE3	2.49	0.48
70:1B:203:PC1:H3F1	69:1B:204:3PE:H3I1	1.96	0.48
5:1E:191:PHE:N	5:1E:194:GLU:OE1	2.47	0.48
7:1G:27:LEU:HD21	7:1G:39:ARG:HH22	1.78	0.48
8:1H:173:TRP:CD1	70:1H:404:PC1:H142	2.49	0.48
10:1J:88:THR:HB	11:1K:23:ARG:NH2	2.28	0.48
11:1K:1:FME:SD	14:1N:79:LEU:HD21	2.52	0.48
12:1L:310:LEU:HA	12:1L:313:MET:HE3	1.96	0.48
14:1N:238:PRO:HB2	69:1N:401:3PE:C1	2.44	0.48
17:1Q:27:GLU:HA	17:1Q:30:ILE:HG22	1.96	0.48
17:1Q:77:ASP:OD1	17:1Q:77:ASP:N	2.34	0.48
24:1Y:45:PRO:HB3	24:1Y:50:GLU:HB3	1.94	0.48
24:1Y:117:MET:CG	70:1Y:206:PC1:H3C2	2.37	0.48
33:1h:70:PRO:HB2	70:1h:202:PC1:H231	1.95	0.48
42:1q:78:ASP:OD1	42:1q:81:MET:HG3	2.13	0.48
46:3B:86:THR:O	46:3B:90:GLU:HG2	2.13	0.48
47:3C:63:PHE:O	47:3C:67:THR:HG23	2.13	0.48
69:3C:507:3PE:C28	69:3C:508:3PE:H261	2.35	0.48
69:3C:508:3PE:H292	75:3F:201:CDL:H652	1.95	0.48
69:3C:515:3PE:H222	70:3P:509:PC1:H31	1.95	0.48
45:3N:6:GLN:HA	45:3N:9:GLN:NE2	2.28	0.48
45:3N:135:LEU:HD21	45:3N:174:VAL:HG21	1.95	0.48
46:3O:160:LEU:HD12	49:3V:64:LEU:HD13	1.95	0.48
47:3P:49:LEU:O	47:3P:53:MET:HG3	2.13	0.48
48:3Q:220:TYR:CD2	69:3T:103:3PE:H391	2.49	0.48
69:3Q:502:3PE:C2D	69:3Q:503:3PE:H2I3	2.43	0.48
49:3R:227:ASN:N	49:3R:234:TYR:HD1	2.07	0.48
49:3R:234:TYR:O	49:3R:243:TYR:N	2.39	0.48
69:3R:305:3PE:H12	51:3T:25:ALA:N	2.24	0.48
51:3T:64:GLN:HB3	51:3T:68:LYS:HZ2	1.76	0.48
55:4A:239:GLY:O	55:4A:243:VAL:HG23	2.13	0.48
56:4B:61:VAL:HG11	93:4B:303:PSC:H41	1.93	0.48
93:4B:303:PSC:H61	93:4B:303:PSC:O02	2.13	0.48
58:4D:67:SER:HB3	59:4E:106:LEU:HD12	1.96	0.48
2:1B:150:PRO:HD3	4:1D:190:HIS:CD2	2.49	0.48
7:1G:456:SER:HB3	7:1G:495:ARG:HD3	1.96	0.48
7:1G:521:VAL:HG22	7:1G:542:PHE:HB3	1.95	0.48
7:1G:601:ARG:NH1	7:1G:605:GLU:OE1	2.45	0.48
9:1I:41:LEU:O	9:1I:41:LEU:HG	2.14	0.48
12:1L:211:MET:HG3	69:1L:711:3PE:H351	1.96	0.48
23:1X:126:LYS:HE3	27:1b:66:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1d:206:3PE:H382	69:1f:104:3PE:C29	2.43	0.48
33:1h:79:PHE:HB3	70:1h:203:PC1:H2	1.96	0.48
69:1o:201:3PE:H232	69:1o:201:3PE:C32	2.40	0.48
42:1q:68:MET:HG2	42:1q:115:PHE:CE2	2.49	0.48
69:3C:504:3PE:H32	69:3C:505:3PE:H251	1.96	0.48
69:3G:103:3PE:H282	69:3G:104:3PE:H222	1.96	0.48
45:3N:284:TYR:CD2	49:3V:71:ASN:HA	2.49	0.48
46:3O:354:ASN:HD21	46:3O:358:GLN:HE21	1.61	0.48
46:3O:382:VAL:HG22	46:3O:392:TYR:CE1	2.48	0.48
47:3P:326:TRP:NE1	51:3T:48:VAL:HG22	2.29	0.48
49:3R:156:LEU:HA	49:3R:269:ASP:OD1	2.14	0.48
55:4A:254:ILE:HG13	55:4A:344:PHE:CD1	2.49	0.48
55:4A:266:GLU:HB3	60:4F:68:THR:HG21	1.96	0.48
59:4E:67:ILE:HA	59:4E:70:VAL:HG12	1.96	0.48
5:1E:154:VAL:HG22	5:1E:155:GLN:N	2.28	0.48
6:1F:92:TYR:CD1	6:1F:133:ALA:HB3	2.48	0.48
6:1F:149:LEU:O	6:1F:153:ILE:HG13	2.14	0.48
6:1F:360:GLY:O	6:1F:366:ARG:HD3	2.14	0.48
13:1M:443:PRO:HB3	70:1M:501:PC1:H2A1	1.96	0.48
24:1Y:10:ASP:OD1	24:1Y:10:ASP:N	2.41	0.48
69:1Y:215:3PE:H222	69:3P:510:3PE:H242	1.96	0.48
29:1d:82:MET:HB3	29:1d:82:MET:HE3	1.78	0.48
37:1l:134:PRO:HD3	40:1o:56:ASP:HA	1.96	0.48
45:3A:219:LEU:O	45:3A:220:SER:C	2.56	0.48
45:3A:312:ILE:HD12	45:3A:319:LEU:HB2	1.96	0.48
47:3C:45:ILE:HA	85:3C:501:HEM:HMC2	1.96	0.48
47:3C:165:TRP:HA	47:3C:174:THR:HG23	1.94	0.48
48:3D:224:GLU:OE1	48:3D:225:PRO:HD2	2.12	0.48
48:3D:226:PRO:HG3	52:3H:83:LEU:HD22	1.96	0.48
49:3E:231:PHE:CE1	49:3E:242:HIS:HB3	2.47	0.48
49:3I:34:LEU:H	49:3I:34:LEU:HG	1.45	0.48
45:3N:106:LEU:HB3	45:3N:107:PRO:HD3	1.93	0.48
46:3O:76:THR:HG23	46:3O:81:SER:HA	1.96	0.48
69:3P:517:3PE:H392	69:3P:518:3PE:H2E2	1.96	0.48
48:3Q:209:LEU:HD22	69:3Q:504:3PE:H3G2	1.95	0.48
50:3S:28:LYS:HA	50:3S:80:TRP:CD1	2.49	0.48
2:1B:177:TYR:CD1	70:1B:202:PC1:H261	2.48	0.48
6:1F:363:THR:HB	6:1F:364:PRO:HD3	1.96	0.48
6:1F:405:CYS:SG	71:1F:502:SF4:S3	3.04	0.48
8:1H:263:THR:O	8:1H:267:THR:OG1	2.27	0.48
8:1H:312:ALA:HB3	25:1Z:55:ARG:HH21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:119:LYS:NZ	75:1L:704:CDL:OA9	2.24	0.48
12:1L:154:LEU:HD13	12:1L:243:VAL:HG22	1.95	0.48
12:1L:533:MET:CE	69:1L:701:3PE:H392	2.44	0.48
69:1L:709:3PE:C3A	75:1i:201:CDL:H771	2.43	0.48
13:1M:95:TYR:HD1	13:1M:136:TRP:CD2	2.32	0.48
19:1S:63:LYS:HG2	19:1S:75:ASN:HB2	1.96	0.48
24:1Y:87:LEU:HD22	69:1Y:212:3PE:C31	2.43	0.48
25:1Z:56:GLU:OE1	25:1Z:59:ARG:NH2	2.36	0.48
38:1m:92:PHE:CA	69:1m:203:3PE:H291	2.44	0.48
38:1m:117:GLU:HB2	38:1m:119:LYS:HE3	1.96	0.48
75:3A:501:CDL:H542	69:3A:503:3PE:H281	1.95	0.48
47:3C:112:THR:O	47:3C:196:HIS:CD2	2.67	0.48
69:3C:515:3PE:H361	70:3P:509:PC1:H242	1.95	0.48
49:3E:207:LYS:C	49:3E:209:GLU:N	2.71	0.48
50:3F:87:LEU:HB3	50:3F:88:PRO:CD	2.43	0.48
46:3O:111:CYS:SG	46:3O:112:LEU:N	2.82	0.48
47:3P:368:ILE:HG21	69:3P:515:3PE:H2B2	1.94	0.48
48:3Q:34:LYS:NZ	48:3Q:34:LYS:HB2	2.28	0.48
49:3R:150:SER:HB3	49:3R:170:ARG:CA	2.44	0.48
49:3R:210:TRP:CD1	49:3R:268:ASP:HB3	2.49	0.48
49:3R:228:ALA:N	49:3R:233:GLY:O	2.35	0.48
52:3U:32:LYS:O	52:3U:36:ARG:HD3	2.13	0.48
69:3W:103:3PE:H121	69:3W:103:3PE:H222	1.96	0.48
69:3X:105:3PE:O22	69:3X:105:3PE:H12	2.13	0.48
55:4A:289:ALA:HB3	55:4A:305:PHE:CD1	2.48	0.48
61:4G:50:TYR:HB2	61:4G:53:LEU:HD12	1.95	0.48
1:1A:69:ILE:HD11	8:1H:144:VAL:HG13	1.95	0.48
6:1F:68:ARG:HD2	6:1F:254:LYS:HG3	1.95	0.48
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.96	0.48
9:1I:53:GLU:OE1	42:1q:34:ARG:NH2	2.47	0.48
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.49	0.48
12:1L:267:MET:HE3	12:1L:267:MET:HB2	1.71	0.48
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	1.96	0.48
23:1X:22:SER:OG	23:1X:89:ASP:OD1	2.26	0.48
82:1Y:203:PGT:H381	82:1Y:203:PGT:H352	1.51	0.48
75:1d:202:CDL:HB62	69:1f:104:3PE:H231	1.96	0.48
69:1d:203:3PE:H351	69:1d:203:3PE:H381	1.62	0.48
32:1g:59:ARG:HB3	75:1g:201:CDL:H131	1.96	0.48
75:1g:201:CDL:H742	33:1h:34:ILE:HB	1.96	0.48
69:1m:202:3PE:H222	69:3T:103:3PE:H291	1.96	0.48
45:3A:40:TRP:CZ2	45:3A:377:GLU:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:242:ARG:NH2	45:3A:431:LEU:O	2.47	0.48
47:3C:158:THR:HA	47:3C:161:VAL:HG12	1.96	0.48
48:3D:221:GLY:O	48:3D:239:PRO:HD2	2.14	0.48
49:3E:102:SER:O	49:3E:105:GLU:HG2	2.13	0.48
51:3G:20:LEU:HD23	51:3G:25:GLN:HB3	1.95	0.48
47:3P:277:ALA:HB1	47:3P:294:LEU:HG	1.95	0.48
69:3P:503:3PE:H2H2	69:3P:518:3PE:H3H1	1.96	0.48
75:3P:513:CDL:H391	69:3P:519:3PE:H2E1	1.96	0.48
69:3P:517:3PE:H32	69:3P:518:3PE:H252	1.96	0.48
49:3R:235:TYR:CD1	49:3R:235:TYR:C	2.92	0.48
69:3W:102:3PE:H252	69:3W:102:3PE:C38	2.33	0.48
54:3Y:6:LEU:HD21	69:3Y:107:3PE:H2D1	1.94	0.48
69:3Y:101:3PE:H2B2	69:3Y:101:3PE:C38	2.44	0.48
55:4A:110:LEU:HA	91:4A:609:PGV:H181	1.95	0.48
56:4B:57:ASP:O	93:4B:303:PSC:O13	2.32	0.48
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.23	0.47
6:1F:305:PRO:HD3	6:1F:413:TRP:HB3	1.95	0.47
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.28	0.47
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.14	0.47
13:1M:150:LEU:HG	13:1M:154:LEU:HD12	1.96	0.47
24:1Y:25:THR:CG2	75:1Y:217:CDL:H411	2.44	0.47
75:1Y:217:CDL:H202	70:3T:102:PC1:C33	2.33	0.47
75:1d:205:CDL:H352	75:1d:205:CDL:H542	1.96	0.47
70:1h:202:PC1:H361	69:1h:204:3PE:H361	1.96	0.47
37:1l:82:ASP:N	37:1l:82:ASP:OD1	2.47	0.47
38:1m:112:GLU:O	38:1m:116:GLN:HG2	2.14	0.47
42:1q:68:MET:HG2	42:1q:115:PHE:CD2	2.49	0.47
47:3C:278:TYR:CE2	47:3C:282:ARG:HD3	2.48	0.47
47:3C:363:LEU:HD12	69:3C:512:3PE:C2H	2.44	0.47
69:3C:516:3PE:H392	69:3C:516:3PE:H2C2	1.96	0.47
69:3N:503:3PE:H322	70:3R:303:PC1:C31	2.44	0.47
46:3O:296:TYR:OH	49:3V:52:ARG:HG2	2.14	0.47
69:3P:506:3PE:O32	69:3P:506:3PE:H261	2.14	0.47
75:3P:513:CDL:H862	75:3P:513:CDL:H662	1.95	0.47
48:3Q:133:GLY:O	48:3Q:151:PRO:HD2	2.14	0.47
55:4A:232:GLN:NE2	56:4B:160:LEU:HD21	2.29	0.47
55:4A:301:THR:HG21	91:4N:101:PGV:H032	1.96	0.47
57:4C:54:MET:CE	91:4C:305:PGV:H132	2.44	0.47
3:1C:71:GLN:OE1	21:1V:82:GLN:NE2	2.47	0.47
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.24	0.47
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.34	0.47
5:1E:6:LEU:O	5:1E:92:ARG:NH2	2.47	0.47
6:1F:90:PRO:O	6:1F:218:CYS:HB2	2.14	0.47
6:1F:357:GLU:O	6:1F:358:SER:C	2.56	0.47
10:1J:115:ILE:CD1	11:1K:6:MET:HE3	2.44	0.47
69:1J:201:3PE:H341	69:1J:201:3PE:H251	1.97	0.47
11:1K:12:PHE:CG	14:1N:72:MET:HE3	2.49	0.47
12:1L:435:PRO:HB3	12:1L:437:PHE:CZ	2.49	0.47
12:1L:602:PHE:CZ	69:1L:706:3PE:C31	2.97	0.47
69:1L:702:3PE:H291	34:1i:80:ILE:CG2	2.39	0.47
13:1M:201:MET:CG	82:1Y:203:PGT:H422	2.44	0.47
14:1N:11:MET:HE1	75:1N:402:CDL:C41	2.43	0.47
16:1P:134:HIS:HB2	16:1P:149:LYS:HD3	1.96	0.47
28:1c:41:GLU:OE1	29:1d:19:ARG:NH2	2.47	0.47
34:1i:54:ALA:O	34:1i:58:ASN:N	2.42	0.47
34:1i:100:LYS:NZ	41:1p:116:GLU:OE1	2.40	0.47
45:3A:49:ASN:OD1	45:3A:51:LYS:HG2	2.14	0.47
45:3A:108:LYS:O	45:3A:112:LEU:HG	2.13	0.47
45:3A:284:TYR:CD2	45:3A:290:MET:HE1	2.48	0.47
46:3B:111:CYS:SG	46:3B:119:LEU:HG	2.54	0.47
46:3B:157:ALA:O	46:3B:161:GLU:HG2	2.14	0.47
69:3G:109:3PE:H3I1	69:3G:109:3PE:H2E2	1.96	0.47
46:3O:124:LEU:HB3	46:3O:223:PHE:CG	2.48	0.47
47:3P:14:ILE:HG13	47:3P:15:ASN:N	2.28	0.47
47:3P:306:MET:CE	69:3P:514:3PE:H272	2.33	0.47
69:3X:108:3PE:H2G1	69:3X:108:3PE:H3F1	1.95	0.47
69:3Y:104:3PE:C3H	75:3Y:106:CDL:H812	2.44	0.47
55:4A:390:MET:HE2	55:4A:390:MET:HA	1.97	0.47
56:4B:188:ARG:HH11	63:4I:51:TYR:HH	1.62	0.47
57:4C:159:MET:SD	57:4C:222:GLN:HG2	2.53	0.47
57:4C:171:VAL:O	57:4C:175:LEU:HG	2.13	0.47
66:4L:14:SER:OG	66:4L:16:GLU:OE1	2.27	0.47
4:1D:71:GLU:OE1	8:1H:134:ARG:NH2	2.46	0.47
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.15	0.47
10:1J:119:PHE:CD1	11:1K:6:MET:HB2	2.50	0.47
10:1J:155:ILE:HD11	70:1J:202:PC1:H361	1.97	0.47
69:1L:703:3PE:H11	69:1k:101:3PE:H392	1.97	0.47
13:1M:90:THR:HG22	13:1M:94:LEU:HD12	1.97	0.47
69:1N:401:3PE:H2E2	69:1N:401:3PE:H3I2	1.96	0.47
69:1d:206:3PE:H2D2	69:1f:104:3PE:C2F	2.44	0.47
45:3A:412:SER:O	53:3J:16:ARG:NH2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3E:249:ILE:HG23	49:3E:249:ILE:O	2.14	0.47
69:3J:104:3PE:H3H1	69:3J:104:3PE:H2E1	1.95	0.47
69:3Q:503:3PE:H332	69:3Q:503:3PE:H242	1.97	0.47
57:4C:98:PHE:HE1	57:4C:252:LEU:HD12	1.79	0.47
58:4D:129:ALA:HB1	58:4D:133:GLY:HA3	1.96	0.47
1:1A:19:LEU:HD11	70:1A:202:PC1:H271	1.96	0.47
3:1C:109:THR:OG1	3:1C:110:TYR:N	2.47	0.47
5:1E:160:TYR:O	5:1E:185:GLY:N	2.44	0.47
5:1E:194:GLU:HA	6:1F:26:TYR:HE2	1.79	0.47
7:1G:94:MET:HE1	7:1G:119:GLN:HB2	1.97	0.47
10:1J:99:MET:HE2	69:1J:201:3PE:C3F	2.35	0.47
14:1N:243:LEU:HD22	14:1N:330:ILE:HG21	1.97	0.47
70:1Y:202:PC1:C21	69:1m:201:3PE:H331	2.44	0.47
70:1Y:206:PC1:H272	70:1Y:206:PC1:H2A1	1.55	0.47
75:1d:205:CDL:H771	75:1d:205:CDL:H231	1.96	0.47
31:1f:22:PHE:CE2	69:1f:104:3PE:C35	2.97	0.47
34:1i:88:HIS:HE1	75:1i:201:CDL:OB3	1.96	0.47
38:1m:106:THR:O	38:1m:110:LYS:HG2	2.15	0.47
45:3A:388:ARG:HH22	45:3A:394:GLU:CD	2.23	0.47
46:3B:170:ASN:CG	46:3B:171:ALA:N	2.72	0.47
46:3B:279:LEU:HA	46:3B:294:SER:OG	2.14	0.47
47:3C:104:TYR:CD1	47:3C:208:PRO:HA	2.50	0.47
69:3C:506:3PE:H342	69:3C:506:3PE:H282	1.96	0.47
48:3D:125:CYS:SG	86:3D:501:HEC:CBB	3.03	0.47
48:3D:249:MET:HB2	86:3D:501:HEC:C1D	2.45	0.47
49:3E:242:HIS:CG	49:3E:251:LYS:HB3	2.49	0.47
45:3N:186:VAL:HG13	45:3N:190:TYR:HB2	1.96	0.47
75:3N:502:CDL:H351	75:3N:502:CDL:H322	1.58	0.47
46:3O:165:ALA:O	46:3O:240:ARG:HD3	2.15	0.47
4:1D:90:LEU:HD13	4:1D:102:TYR:OH	2.15	0.47
5:1E:76:PRO:HB2	5:1E:79:ARG:HG2	1.96	0.47
5:1E:143:GLU:HG3	6:1F:356:HIS:CD2	2.50	0.47
6:1F:120:GLU:HG3	6:1F:232:PRO:HG2	1.96	0.47
6:1F:224:ASN:ND2	73:1F:501:FMN:O2	2.47	0.47
10:1J:101:PHE:CD1	10:1J:101:PHE:C	2.92	0.47
11:1K:59:MET:HG2	14:1N:27:LEU:HD22	1.96	0.47
13:1M:94:LEU:HD21	69:1N:401:3PE:C23	2.44	0.47
69:1N:401:3PE:H12	69:1N:401:3PE:HN2	1.79	0.47
69:1d:201:3PE:H2H2	69:1d:201:3PE:H2E2	1.64	0.47
75:1d:202:CDL:CB6	69:1f:104:3PE:H231	2.45	0.47
69:1d:206:3PE:C37	69:1f:104:3PE:C29	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:21:VAL:HG21	69:1f:104:3PE:H3G1	1.95	0.47
69:1f:103:3PE:H261	69:1f:104:3PE:H3I2	1.96	0.47
34:1i:82:HIS:NE2	41:1p:41:ASP:OD1	2.40	0.47
75:1i:201:CDL:H601	41:1p:43:PRO:HB2	1.96	0.47
69:1k:101:3PE:N	69:1o:201:3PE:H222	2.29	0.47
37:1l:81:LEU:O	37:1l:85:ILE:HG23	2.15	0.47
39:1n:153:LEU:HD13	39:1n:165:LEU:HB2	1.96	0.47
45:3A:156:THR:HA	49:3E:85:VAL:HG21	1.97	0.47
45:3A:304:CYS:HB2	45:3A:325:VAL:O	2.15	0.47
47:3C:359:PHE:HD2	69:3C:511:3PE:H3A1	1.80	0.47
47:3C:368:ILE:CG2	69:3C:507:3PE:C27	2.93	0.47
69:3C:513:3PE:H332	69:3X:107:3PE:H262	1.96	0.47
48:3D:96:PRO:CG	52:3H:91:ASP:HB3	2.43	0.47
49:3E:204:ARG:NH1	49:3E:246:SER:O	2.47	0.47
49:3E:233:GLY:HA3	49:3E:245:ALA:N	2.29	0.47
45:3N:207[B]:GLN:HA	45:3N:210:ASP:OD2	2.15	0.47
69:3N:501:3PE:H381	75:3N:502:CDL:H312	1.96	0.47
47:3P:8:HIS:CD2	47:3P:10:LEU:H	2.33	0.47
47:3P:126:THR:HG22	47:3P:182:HIS:CE1	2.50	0.47
48:3Q:147:LEU:CD2	48:3Q:157:ALA:HB1	2.45	0.47
53:3W:38:GLN:HG2	69:3W:102:3PE:O22	2.14	0.47
87:3X:102:PEK:N	60:4F:1:ALA:CB	2.62	0.47
54:3Y:51:LYS:O	54:3Y:51:LYS:HG2	2.14	0.47
75:3Y:106:CDL:H542	75:3Y:106:CDL:C11	2.44	0.47
75:3Y:106:CDL:H412	69:3Y:107:3PE:H2F2	1.97	0.47
55:4A:404:THR:HG21	67:4M:3:ALA:HB2	1.97	0.47
55:4A:409:TRP:CE2	91:4A:606:PGV:H52	2.50	0.47
57:4C:99:TRP:CD1	91:4C:303:PGV:H42	2.50	0.47
59:4E:19:PHE:O	59:4E:57:ARG:NH2	2.47	0.47
2:1B:77:ARG:HA	2:1B:77:ARG:HD2	1.65	0.47
3:1C:90:PHE:HZ	3:1C:163:ARG:HE	1.63	0.47
4:1D:19:MET:HE2	14:1N:173:THR:HG22	1.96	0.47
5:1E:106:THR:HG23	5:1E:110:LEU:HD21	1.97	0.47
5:1E:109:MET:C	5:1E:111:ARG:N	2.71	0.47
6:1F:308:PRO:HD3	6:1F:421:HIS:CD2	2.50	0.47
7:1G:351:THR:O	7:1G:351:THR:OG1	2.27	0.47
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.50	0.47
75:1H:401:CDL:HB61	75:1H:401:CDL:H332	1.96	0.47
9:1I:53:GLU:CG	42:1q:61:TRP:HB3	2.44	0.47
11:1K:14:ILE:HD12	11:1K:15:ALA:N	2.29	0.47
12:1L:2:ASN:OD1	12:1L:2:ASN:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1L:706:3PE:C11	24:1Y:2:LYS:NZ	2.78	0.47
69:1N:401:3PE:H2B2	69:1N:401:3PE:H281	1.68	0.47
17:1Q:36:ARG:NH1	17:1Q:106:GLU:OE2	2.47	0.47
24:1Y:107:TYR:CD2	69:1Y:213:3PE:O11	2.68	0.47
75:1d:202:CDL:H512	75:1d:202:CDL:OB8	2.15	0.47
32:1g:63:PHE:CD2	75:1g:201:CDL:H172	2.50	0.47
32:1g:88:TRP:O	32:1g:92:GLU:HG3	2.15	0.47
75:1q:201:CDL:H542	75:1q:201:CDL:H511	1.79	0.47
75:1q:202:CDL:H252	75:1q:202:CDL:C42	2.41	0.47
43:1r:15:SER:OG	43:1r:19:LEU:HD23	2.15	0.47
45:3A:141:ASN:C	45:3A:143:SER:N	2.70	0.47
69:3A:502:3PE:H272	70:3J:106:PC1:H241	1.95	0.47
69:3A:502:3PE:H282	69:3E:302:3PE:H2H1	1.97	0.47
49:3E:205:VAL:HG12	49:3E:207:LYS:O	2.14	0.47
49:3E:212:ILE:HG21	49:3E:273:VAL:CG2	2.44	0.47
51:3G:41:ARG:HD3	69:3G:107:3PE:H121	1.96	0.47
45:3N:223:TYR:CE1	45:3N:229:PRO:HD2	2.49	0.47
47:3P:10:LEU:HB3	47:3P:11:MET:HE2	1.97	0.47
47:3P:284:ILE:HG13	47:3P:290:GLY:HA2	1.95	0.47
69:3P:508:3PE:H382	69:3P:508:3PE:C3C	2.44	0.47
48:3Q:118:ARG:CG	48:3Q:194:SER:HB3	2.37	0.47
48:3Q:180:SER:HB2	52:3U:77:LEU:HD11	1.97	0.47
49:3R:160:PRO:HD2	49:3R:163:LYS:CB	2.38	0.47
53:3W:56:ILE:CG1	53:3W:57:LYS:HG3	2.44	0.47
69:3X:101:3PE:H281	69:3X:101:3PE:H252	1.69	0.47
75:3X:103:CDL:H241	75:3X:103:CDL:C87	2.43	0.47
70:3X:104:PC1:H2D1	70:3X:104:PC1:H2A1	1.51	0.47
69:3X:108:3PE:H2D1	69:3X:108:3PE:H3E2	1.95	0.47
91:4A:607:PGV:H151	68:4N:22:ILE:CG2	2.44	0.47
57:4C:251:PHE:HE1	91:4C:303:PGV:H161	1.80	0.47
58:4D:122:ARG:HG3	65:4K:53:TRP:CE2	2.50	0.47
1:1A:17:LEU:HB3	8:1H:222:MET:SD	2.54	0.47
7:1G:218:ARG:HD2	7:1G:220:TRP:CH2	2.49	0.47
7:1G:544:ILE:HG23	7:1G:559:VAL:HG23	1.96	0.47
8:1H:172:ILE:HG12	8:1H:176:PHE:CD2	2.49	0.47
12:1L:19:ILE:HD12	12:1L:123:LEU:HG	1.96	0.47
12:1L:120:TYR:OH	75:1L:704:CDL:OB3	2.33	0.47
75:1L:704:CDL:O1	13:1M:357:THR:OG1	2.20	0.47
14:1N:242:SER:HB3	69:1N:401:3PE:C24	2.44	0.47
16:1P:196:LEU:HB3	16:1P:198:LYS:HG2	1.97	0.47
20:1U:36:PHE:HB3	20:1U:42:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:25:THR:HG21	75:1Y:217:CDL:H411	1.96	0.47
24:1Y:72:THR:HA	69:1Y:214:3PE:H281	1.96	0.47
69:1g:202:3PE:H391	69:1g:202:3PE:H362	1.68	0.47
33:1h:109:GLU:OE1	33:1h:109:GLU:HA	2.15	0.47
70:1h:203:PC1:H351	70:1h:203:PC1:H382	1.65	0.47
34:1i:83:TYR:CB	75:1i:201:CDL:H531	2.44	0.47
34:1i:88:HIS:NE2	75:1i:201:CDL:OB2	2.43	0.47
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.15	0.47
69:3A:502:3PE:H362	69:3A:502:3PE:C26	2.42	0.47
47:3C:284:ILE:HD13	69:3C:512:3PE:H261	1.97	0.47
47:3C:364:VAL:HG13	69:3C:506:3PE:H2B1	1.95	0.47
49:3E:173:PRO:HD2	49:3E:216:VAL:CG2	2.45	0.47
49:3E:254:ALA:HB1	49:3E:255:PRO:CD	2.45	0.47
69:3E:303:3PE:H2C2	69:3E:303:3PE:H3F1	1.97	0.47
51:3G:63:TRP:CD1	69:3G:110:3PE:H221	2.50	0.47
69:3G:109:3PE:C2I	69:3G:110:3PE:H371	2.45	0.47
53:3J:45:GLU:OE2	53:3J:54:LYS:HE2	2.15	0.47
53:3J:54:LYS:H	53:3J:57:LYS:HB2	1.80	0.47
45:3N:135:LEU:CD2	45:3N:174:VAL:HG21	2.45	0.47
69:3N:503:3PE:H271	70:3R:303:PC1:O32	2.15	0.47
46:3O:306:PRO:HA	49:3V:52:ARG:HD3	1.96	0.47
47:3P:285:PRO:CG	69:3P:517:3PE:O14	2.63	0.47
69:3P:504:3PE:C35	69:3Y:103:3PE:H351	2.44	0.47
69:3P:508:3PE:C33	75:3P:513:CDL:H131	2.29	0.47
49:3R:133:VAL:O	49:3R:137:VAL:HG23	2.13	0.47
49:3R:178:HIS:CD2	49:3R:210:TRP:HE1	2.33	0.47
49:3R:204:ARG:HB3	49:3R:204:ARG:NH1	2.30	0.47
49:3R:230:ASP:OD1	49:3R:231:PHE:N	2.48	0.47
51:3T:42:ARG:HB3	70:3T:102:PC1:H152	1.96	0.47
69:3W:103:3PE:H351	54:3X:23:MET:CE	2.33	0.47
69:3W:103:3PE:H271	91:4C:302:PGV:H22	1.95	0.47
69:3Y:102:3PE:H2B1	69:3Y:105:3PE:H111	1.96	0.47
75:3Y:106:CDL:HA21	75:3Y:106:CDL:H111	1.97	0.47
55:4A:13:LYS:HE2	55:4A:500:PRO:HB2	1.95	0.47
55:4A:48:LEU:O	55:4A:48:LEU:HD12	2.14	0.47
57:4C:107:ALA:HB3	91:4C:303:PGV:O11	2.15	0.47
75:4C:307:CDL:HA62	64:4J:2:GLU:H	1.80	0.47
1:1A:23:TRP:CZ2	70:1A:202:PC1:O12	2.59	0.47
4:1D:100:LEU:HD13	4:1D:196:PRO:HD3	1.95	0.47
5:1E:106:THR:CG2	5:1E:110:LEU:HD21	2.45	0.47
8:1H:70:MET:HE2	8:1H:121:TRP:CE3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:195:ARG:HH21	8:1H:274:ARG:HG3	1.79	0.47
12:1L:80:PHE:CZ	75:1i:201:CDL:H402	2.50	0.47
12:1L:358:LYS:HG3	39:1n:79:TYR:CE1	2.50	0.47
69:1L:711:3PE:H12	69:1M:502:3PE:H121	1.96	0.47
13:1M:108:MET:CB	13:1M:121:LEU:HD13	2.45	0.47
13:1M:130:LEU:HD22	13:1M:150:LEU:HD13	1.97	0.47
19:1S:18:ILE:HD11	19:1S:52:ILE:HG12	1.97	0.47
20:1T:34:SER:H	20:1T:73:PRO:HD2	1.78	0.47
21:1V:93:MET:SD	21:1V:98:PRO:HG2	2.55	0.47
24:1Y:78:GLN:CD	51:3T:56:TYR:OH	2.55	0.47
33:1h:80:TYR:H	70:1h:203:PC1:H121	1.79	0.47
45:3A:93:GLU:HG3	45:3A:94:HIS:CD2	2.50	0.47
46:3B:294:SER:HB2	46:3B:343:GLN:NE2	2.30	0.47
69:3C:515:3PE:H342	69:3C:515:3PE:C39	2.44	0.47
69:3C:516:3PE:H3B1	69:3C:516:3PE:H371	1.95	0.47
48:3D:146:GLU:HG2	48:3D:175:LEU:HD11	1.96	0.47
51:3G:52:PRO:HB2	51:3G:53:PRO:HD3	1.96	0.47
45:3N:133:VAL:HG11	49:3V:53:GLU:OE1	2.15	0.47
45:3N:209:LEU:HG	45:3N:213:GLN:HE21	1.80	0.47
46:3O:338:LYS:HE2	46:3O:434:PRO:HG3	1.96	0.47
47:3P:43:LEU:C	47:3P:43:LEU:HD23	2.40	0.47
47:3P:221:HIS:HA	47:3P:225:THR:CG2	2.45	0.47
48:3Q:123:GLY:O	48:3Q:127:VAL:HG23	2.15	0.47
60:4F:49:VAL:HG23	60:4F:91:LEU:HD12	1.97	0.47
61:4G:44:ARG:HH12	61:4G:84:GLN:HB3	1.80	0.47
70:1H:402:PC1:H3F1	27:1b:24:ILE:HD13	1.93	0.47
12:1L:588:PHE:CZ	14:1N:62:THR:HG22	2.50	0.47
69:1L:706:3PE:C11	24:1Y:2:LYS:HZ1	2.28	0.47
13:1M:12:LEU:HD22	13:1M:97:THR:HG23	1.96	0.47
13:1M:145:ALA:HB1	13:1M:219:ALA:HA	1.96	0.47
14:1N:256:PRO:HB2	69:1N:401:3PE:H2H2	1.96	0.47
75:1N:402:CDL:H611	75:1N:402:CDL:H772	1.97	0.47
69:1Y:215:3PE:H342	69:3P:510:3PE:H3D1	1.95	0.47
29:1d:71:PHE:HE2	75:1d:205:CDL:H642	1.80	0.47
31:1f:10:HIS:O	69:1f:101:3PE:C2G	2.62	0.47
37:1l:99:ASN:HB2	38:1m:6:LYS:HE2	1.96	0.47
40:1o:68:CYS:O	40:1o:72:SER:N	2.47	0.47
45:3A:62:LEU:HD11	45:3A:127:ILE:HG12	1.97	0.47
47:3C:138:MET:HE1	47:3C:267:HIS:O	2.14	0.47
69:3C:513:3PE:C32	69:3C:517:3PE:H32	2.45	0.47
48:3D:309:TYR:CZ	48:3D:313:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3F:44:MET:HA	50:3F:98:ASP:OD1	2.14	0.47
69:3G:106:3PE:H321	69:3G:106:3PE:H352	1.57	0.47
53:3J:23:LEU:CD2	69:3J:103:3PE:H3A2	2.44	0.47
45:3N:303:LEU:HD21	45:3N:333:ASP:HB3	1.97	0.47
47:3P:131:TYR:O	47:3P:134:PRO:HD2	2.14	0.47
48:3Q:72:ASP:HB2	48:3Q:83:ARG:HG2	1.97	0.47
48:3Q:109:LEU:HD12	48:3Q:110:PRO:HD2	1.96	0.47
49:3R:179:ARG:HG2	49:3R:245:ALA:HB1	1.97	0.47
69:3Y:101:3PE:H382	69:3Y:101:3PE:H3B1	1.50	0.47
56:4B:52:HIS:HD2	59:4E:40:ASP:N	2.13	0.47
56:4B:65:TRP:HB3	93:4B:303:PSC:C13	2.42	0.47
59:4E:27:TRP:CH2	59:4E:31:LYS:HD3	2.50	0.47
1:1A:103:ALA:CB	69:1b:101:3PE:C35	2.92	0.47
6:1F:342:ASP:OD1	6:1F:429:ARG:NH2	2.43	0.47
8:1H:175:ILE:HG23	8:1H:176:PHE:N	2.30	0.47
8:1H:222:MET:HA	8:1H:222:MET:HE2	1.97	0.47
10:1J:91:GLY:CA	69:1J:201:3PE:H362	2.40	0.47
11:1K:12:PHE:CZ	14:1N:72:MET:HB2	2.49	0.47
12:1L:194:ASN:ND2	41:1p:106:GLN:OE1	2.48	0.47
12:1L:205:ASN:HB3	41:1p:121:ARG:HH12	1.80	0.47
14:1N:7:THR:HG21	75:1N:402:CDL:C34	2.37	0.47
19:1S:32:VAL:HA	19:1S:86:VAL:HG21	1.96	0.47
24:1Y:35:VAL:HG21	69:1Y:208:3PE:H221	1.97	0.47
24:1Y:39:SER:OG	69:1Y:204:3PE:H11	2.15	0.47
70:1Y:207:PC1:H2E2	69:1Y:213:3PE:H361	1.96	0.47
27:1b:26:GLY:HA3	69:1b:101:3PE:H291	1.97	0.47
31:1f:31:ASP:OD1	31:1f:32:GLU:N	2.48	0.47
32:1g:68:ILE:HG23	32:1g:72:LEU:HD12	1.96	0.47
70:1h:202:PC1:H111	70:1h:202:PC1:C2	2.44	0.47
37:1l:112:MET:HE2	37:1l:112:MET:HA	1.95	0.47
47:3C:38:GLY:O	47:3C:42:ILE:HG13	2.14	0.47
47:3C:262:LEU:HD11	49:3R:172:LYS:HA	1.97	0.47
48:3D:125:CYS:SG	86:3D:501:HEC:CAB	3.03	0.47
69:3P:508:3PE:C39	75:3P:513:CDL:H372	2.45	0.47
69:3P:520:3PE:C3A	69:3Q:504:3PE:H361	2.45	0.47
69:3Q:503:3PE:H372	69:3Q:503:3PE:H282	1.96	0.47
54:3X:36:THR:O	54:3X:37:ASP:C	2.58	0.47
54:3Y:23:MET:O	54:3Y:27:VAL:HG23	2.14	0.47
55:4A:190:ILE:O	55:4A:194:LEU:HD12	2.14	0.47
55:4A:289:ALA:HA	55:4A:292:MET:HE2	1.95	0.47
57:4C:204:HIS:NE2	57:4C:249:TRP:HB2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4D:119:GLN:O	58:4D:123:MET:HG3	2.15	0.47
6:1F:101:GLU:HG3	6:1F:184:TYR:CE1	2.48	0.46
7:1G:56:LEU:HD12	7:1G:67:ALA:CA	2.46	0.46
12:1L:534:HIS:ND1	69:1L:701:3PE:P	2.88	0.46
13:1M:281:ASP:OD1	13:1M:340:ARG:HB3	2.15	0.46
15:1O:320:LYS:O	29:1d:60:ARG:NH2	2.48	0.46
16:1P:134:HIS:NE2	16:1P:169:SER:O	2.47	0.46
24:1Y:4:LEU:HD11	24:1Y:26:SER:HB3	1.97	0.46
24:1Y:6:HIS:O	24:1Y:10:ASP:OD1	2.34	0.46
31:1f:22:PHE:CZ	69:1f:104:3PE:H351	2.50	0.46
75:1g:201:CDL:HA22	33:1h:27:PHE:CD2	2.50	0.46
69:1k:101:3PE:H112	69:1o:201:3PE:H222	1.96	0.46
69:1l:202:3PE:O22	69:1l:202:3PE:H11	2.15	0.46
41:1p:73:ILE:HG23	41:1p:155:LEU:HD22	1.97	0.46
45:3A:3:THR:O	45:3A:5:ALA:N	2.44	0.46
46:3B:170:ASN:CG	46:3B:171:ALA:H	2.23	0.46
46:3B:242:GLY:O	46:3B:423:SER:HA	2.15	0.46
47:3C:24:PRO:HB2	47:3C:27:ILE:HG23	1.97	0.46
47:3C:337:TRP:O	47:3C:341:GLN:HG2	2.14	0.46
69:3C:507:3PE:O21	69:3C:507:3PE:H242	2.15	0.46
69:3C:513:3PE:H381	69:3C:513:3PE:H2B2	1.97	0.46
48:3D:165:ASP:OD1	48:3D:165:ASP:N	2.45	0.46
49:3E:206:LYS:HD2	49:3E:263:TYR:HE1	1.79	0.46
45:3N:124:ASP:OD1	45:3N:179:ARG:HB2	2.15	0.46
46:3O:232:LEU:HD22	46:3O:232:LEU:HA	1.71	0.46
47:3P:119:LEU:O	47:3P:123:VAL:HG23	2.15	0.46
47:3P:129:MET:HE1	47:3P:181:PHE:HB3	1.97	0.46
70:3P:509:PC1:H111	70:3P:509:PC1:H152	1.58	0.46
49:3R:201:ASP:CG	49:3R:202:LEU:N	2.72	0.46
52:3U:27:ILE:O	52:3U:31:ILE:HG12	2.16	0.46
55:4A:208:MET:HE3	57:4C:100:ALA:CB	2.42	0.46
91:4G:102:PGV:H131	91:4G:102:PGV:H102	1.59	0.46
68:4N:40:ASN:CG	91:4N:101:PGV:O06	2.57	0.46
1:1A:23:TRP:CA	70:1A:202:PC1:H121	2.42	0.46
1:1A:30:TYR:OH	2:1B:111:ARG:NH2	2.49	0.46
1:1A:54:LYS:HB3	1:1A:113:TRP:HE3	1.79	0.46
69:1A:201:3PE:H3A1	69:1b:101:3PE:C2A	2.41	0.46
2:1B:32:LYS:HE3	69:1B:205:3PE:O12	2.15	0.46
5:1E:102:VAL:HG22	5:1E:154:VAL:HG23	1.96	0.46
6:1F:125:GLY:O	6:1F:129:MET:HG3	2.16	0.46
7:1G:43:HIS:HD2	7:1G:45:ARG:H	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:673:MET:HG3	7:1G:679:ARG:HG2	1.97	0.46
10:1J:163:ILE:HG21	14:1N:12:THR:HG21	1.96	0.46
12:1L:8:THR:HB	12:1L:82:MET:HE3	1.97	0.46
12:1L:161:ARG:HA	39:1n:91:GLU:HG3	1.97	0.46
15:1O:50:HIS:NE2	15:1O:125:GLU:CD	2.70	0.46
70:1P:502:PC1:H111	70:1P:502:PC1:H153	1.68	0.46
69:1d:201:3PE:C3F	69:1d:201:3PE:H2E2	2.44	0.46
34:1i:103:ILE:HD12	34:1i:103:ILE:C	2.40	0.46
39:1n:130:GLU:N	39:1n:130:GLU:OE2	2.49	0.46
47:3C:25:SER:HB3	47:3C:218:ILE:HG23	1.97	0.46
69:3C:503:3PE:H251	69:3C:505:3PE:H321	1.98	0.46
69:3C:513:3PE:H2A2	69:3C:517:3PE:H372	1.97	0.46
49:3I:62:ARG:HB3	49:3I:63:PRO:HD2	1.97	0.46
45:3N:135:LEU:HA	45:3N:138:LEU:HD12	1.96	0.46
47:3P:114:ASN:ND2	70:3P:509:PC1:O22	2.46	0.46
48:3Q:34:LYS:HG3	48:3Q:35:GLN:HG3	1.96	0.46
49:3R:234:TYR:CB	49:3R:243:TYR:HB2	2.45	0.46
51:3T:73:ASN:OD1	51:3T:74:PRO:HD2	2.16	0.46
52:3U:27:ILE:CG1	52:3U:30:CYS:HB2	2.45	0.46
53:3W:23:LEU:CD2	69:3W:103:3PE:H3A2	2.42	0.46
55:4A:409:TRP:CZ2	91:4A:606:PGV:H52	2.51	0.46
1:1A:21:ALA:HB1	8:1H:218:GLY:CA	2.45	0.46
6:1F:102:PRO:HD2	6:1F:302:SER:HB3	1.96	0.46
7:1G:159:CYS:HA	7:1G:202:ILE:HD11	1.98	0.46
9:1I:95:GLU:HG3	9:1I:108:ARG:HD2	1.97	0.46
10:1J:99:MET:SD	69:1J:203:3PE:H3D1	2.48	0.46
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.31	0.46
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.97	0.46
69:1L:708:3PE:H31	69:1L:708:3PE:H231	1.97	0.46
13:1M:457:PRO:O	32:1g:84:ARG:NH2	2.48	0.46
15:1O:24:VAL:HG13	15:1O:167:HIS:H	1.80	0.46
20:1T:71:MET:HE3	20:1T:71:MET:HB3	1.78	0.46
82:1Y:203:PGT:H341	82:1Y:203:PGT:H131	1.97	0.46
69:1g:203:3PE:H351	69:1g:203:3PE:H252	1.97	0.46
35:1j:38:TRP:CD2	69:1k:101:3PE:H371	2.42	0.46
69:1m:205:3PE:H2A2	69:1m:205:3PE:H272	1.63	0.46
41:1p:48:ARG:HG3	41:1p:52:GLU:HG3	1.97	0.46
41:1p:98:ASP:O	41:1p:102:VAL:HG12	2.15	0.46
47:3C:361:ILE:HA	47:3C:365:LEU:HB2	1.98	0.46
48:3D:120:VAL:HG22	48:3D:258:LEU:HD21	1.96	0.46
45:3N:144:SER:O	45:3N:148:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:3N:502:CDL:H841	75:3X:103:CDL:C81	2.45	0.46
46:3O:129:ALA:H	46:3O:130:PRO:HD3	1.79	0.46
47:3P:8:HIS:CG	47:3P:11:MET:HG2	2.51	0.46
75:3P:513:CDL:H792	51:3T:41:THR:HG21	1.97	0.46
75:3X:103:CDL:HA62	69:3X:105:3PE:O22	2.15	0.46
69:3Y:107:3PE:H242	69:3Y:107:3PE:C2	2.46	0.46
55:4A:217:THR:HG22	57:4C:188:ILE:HG12	1.96	0.46
55:4A:240:HIS:CD2	55:4A:244:TYR:HE2	2.33	0.46
57:4C:83:MET:HG3	57:4C:237:ALA:CB	2.45	0.46
57:4C:92:LEU:O	57:4C:95:THR:OG1	2.30	0.46
57:4C:137:LEU:HD22	57:4C:246:ASP:OD1	2.16	0.46
1:1A:23:TRP:O	70:1A:202:PC1:C12	2.64	0.46
5:1E:154:VAL:HG12	5:1E:161:TYR:HB2	1.98	0.46
6:1F:193:ILE:HG23	6:1F:215:VAL:HA	1.97	0.46
7:1G:199:ILE:CG2	7:1G:208:LEU:HD13	2.45	0.46
10:1J:41:CYS:SG	10:1J:57:PHE:HD2	2.37	0.46
10:1J:99:MET:HE2	69:1J:201:3PE:C3H	2.37	0.46
12:1L:183:VAL:HG21	13:1M:400:MET:HE1	1.98	0.46
12:1L:375:ILE:HD12	12:1L:458:LEU:HD21	1.96	0.46
69:1L:706:3PE:H112	24:1Y:2:LYS:NZ	2.31	0.46
13:1M:336:ARG:O	13:1M:425:ASN:ND2	2.49	0.46
15:1O:36:GLY:O	15:1O:40:ARG:NH1	2.47	0.46
15:1O:187:GLY:O	15:1O:192:MET:HG3	2.16	0.46
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.34	0.46
16:1P:81:ILE:HG21	16:1P:117:ILE:HA	1.96	0.46
20:1T:81:ALA:HA	20:1T:86:VAL:HB	1.98	0.46
21:1V:7:THR:HG23	21:1V:9:GLY:H	1.81	0.46
69:1Y:205:3PE:H291	69:1Y:208:3PE:H2B1	1.98	0.46
27:1b:23:ALA:CB	69:1b:101:3PE:H2G2	2.43	0.46
69:1d:203:3PE:H321	69:1d:203:3PE:H3B1	1.96	0.46
34:1i:17:LEU:HD11	39:1n:162:LEU:HG	1.97	0.46
34:1i:88:HIS:NE2	75:1i:201:CDL:OB3	2.48	0.46
37:1l:127:PRO:HG3	40:1o:3:HIS:CG	2.51	0.46
37:1l:134:PRO:HA	40:1o:57:TYR:CZ	2.50	0.46
38:1m:106:THR:HG21	69:1m:205:3PE:H241	1.97	0.46
40:1o:77:LEU:CG	69:1o:201:3PE:H261	2.45	0.46
41:1p:2:ASP:OD2	41:1p:6:LYS:NZ	2.47	0.46
45:3A:80:GLU:HG2	46:3B:284:HIS:HB2	1.97	0.46
45:3A:280:TYR:HA	45:3A:284:TYR:CE2	2.50	0.46
48:3D:163:ASN:CG	48:3D:164:GLU:H	2.23	0.46
49:3E:200:HIS:CE1	49:3E:202:LEU:H	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:307:PHE:CD1	46:3O:307:PHE:C	2.93	0.46
49:3R:128:ALA:HB1	69:3R:302:3PE:C36	2.38	0.46
49:3R:225:ILE:HG12	49:3R:237:PRO:HG3	1.98	0.46
53:3W:14:LEU:HD22	69:3W:103:3PE:H3C1	1.96	0.46
55:4A:253:MET:HG2	55:4A:396:TRP:CZ3	2.50	0.46
55:4A:423:MET:HE1	91:4K:101:PGV:C34	2.44	0.46
91:4A:609:PGV:C22	91:4A:609:PGV:H51	2.46	0.46
4:1D:83:LEU:O	4:1D:85:ARG:HD2	2.15	0.46
70:1H:402:PC1:C3F	27:1b:24:ILE:CD1	2.88	0.46
12:1L:104:SER:HB2	12:1L:118:PHE:CZ	2.51	0.46
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.15	0.46
13:1M:98:MET:CB	13:1M:132:ILE:HD11	2.45	0.46
24:1Y:65:ILE:HD11	24:1Y:100:LEU:HB2	1.96	0.46
69:1Y:204:3PE:H371	69:1Y:204:3PE:H241	1.97	0.46
25:1Z:85:GLN:O	25:1Z:89:GLU:HB2	2.15	0.46
34:1i:103:ILE:HD11	40:1o:47:ASP:OD2	2.16	0.46
37:1l:106:SER:HG	69:1l:203:3PE:H341	1.78	0.46
69:1m:203:3PE:C3C	69:1m:205:3PE:H3I1	2.45	0.46
40:1o:45:MET:HB2	40:1o:50:LEU:HD22	1.97	0.46
46:3B:122:PHE:O	46:3B:126:VAL:HG13	2.15	0.46
46:3B:275:LEU:HD13	46:3B:410:VAL:HG12	1.98	0.46
46:3B:411:ILE:C	46:3B:412:ASN:CA	2.89	0.46
47:3C:356:ILE:CA	69:3C:511:3PE:H391	2.45	0.46
69:3C:512:3PE:H3A2	69:3C:513:3PE:H291	1.97	0.46
69:3C:515:3PE:H121	70:3P:509:PC1:H121	1.98	0.46
48:3D:329:PRO:HD3	51:3G:14:HIS:CD2	2.49	0.46
49:3E:200:HIS:O	49:3E:203:GLU:HB3	2.15	0.46
49:3E:207:LYS:C	49:3E:209:GLU:H	2.24	0.46
49:3E:223:VAL:HG22	48:3Q:107:GLY:O	2.16	0.46
45:3N:38:GLY:O	45:3N:197:LEU:HD12	2.16	0.46
45:3N:207[A]:GLN:HA	45:3N:210:ASP:OD2	2.15	0.46
45:3N:301:ARG:HD2	47:3P:1:MET:O	2.15	0.46
69:3N:501:3PE:C3B	47:3P:14:ILE:HD11	2.42	0.46
69:3N:501:3PE:C39	69:3P:511:3PE:H3B2	2.44	0.46
47:3P:323:CYS:CB	69:3P:516:3PE:H3H1	2.45	0.46
69:3P:506:3PE:O12	69:3P:506:3PE:C12	2.63	0.46
70:3P:509:PC1:H341	70:3P:509:PC1:H372	1.65	0.46
69:3P:515:3PE:C3I	69:3P:517:3PE:H2B1	2.46	0.46
49:3R:204:ARG:HE	49:3R:257:ASN:ND2	2.13	0.46
50:3S:50:LEU:HD11	50:3S:90:LEU:HD13	1.97	0.46
49:3V:62:ARG:HB3	49:3V:63:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:278:MET:HE1	91:4A:607:PGV:H51	1.97	0.46
75:4B:302:CDL:H652	75:4B:302:CDL:C42	2.46	0.46
87:4G:103:PEK:H8	87:4G:103:PEK:H311	1.98	0.46
1:1A:3:ILE:HG23	1:1A:4:MET:N	2.31	0.46
2:1B:80:PRO:HD3	4:1D:54:GLN:NE2	2.30	0.46
70:1B:203:PC1:H3A1	69:1B:205:3PE:H3F2	1.97	0.46
69:1B:205:3PE:H351	75:1q:202:CDL:H572	1.97	0.46
4:1D:246:THR:HG23	21:1V:12:GLY:HA3	1.96	0.46
6:1F:107:ASP:OD1	6:1F:108:ARG:N	2.49	0.46
8:1H:65:THR:HA	16:1P:324:TYR:HB2	1.98	0.46
10:1J:19:GLY:O	10:1J:24:PRO:HD3	2.15	0.46
10:1J:170:GLU:OE1	10:1J:173:ARG:NH2	2.47	0.46
12:1L:18:PRO:HA	12:1L:35:TYR:HE2	1.81	0.46
12:1L:471:ASN:ND2	69:1o:201:3PE:H2H1	2.30	0.46
13:1M:46:GLY:HA2	32:1g:84:ARG:HG2	1.97	0.46
69:1N:401:3PE:H3G2	69:1N:401:3PE:C2E	2.42	0.46
15:1O:73:LEU:HD23	15:1O:292:VAL:HG13	1.97	0.46
16:1P:266:VAL:O	16:1P:270:PHE:HD1	1.97	0.46
34:1i:71:VAL:HA	34:1i:75:LEU:HB2	1.96	0.46
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.51	0.46
40:1o:75:ASN:CG	69:1o:201:3PE:H252	2.38	0.46
69:3A:502:3PE:H3D2	69:3A:502:3PE:C39	2.42	0.46
46:3B:283:PRO:HD3	49:3I:57:GLY:HA2	1.98	0.46
47:3C:296:ALA:CB	69:3C:511:3PE:H3F2	2.45	0.46
69:3S:201:3PE:H3H1	70:3T:102:PC1:H3D2	1.97	0.46
69:3X:105:3PE:H3B2	69:3X:105:3PE:H281	1.96	0.46
55:4A:28:MET:HE2	67:4M:26:PHE:HE2	1.79	0.46
55:4A:359:ALA:HA	88:4A:602:HEA:OMA	2.16	0.46
88:4A:601:HEA:H171	88:4A:601:HEA:H202	1.75	0.46
57:4C:178:ALA:HB1	91:4C:304:PGV:H21	1.97	0.46
70:1B:202:PC1:H111	16:1P:276:GLU:OE1	2.15	0.46
69:1B:204:3PE:H2B2	69:1B:205:3PE:H291	1.98	0.46
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.97	0.46
4:1D:343:GLU:HG3	7:1G:98:LEU:HD23	1.96	0.46
7:1G:105:CYS:N	7:1G:106:PRO:CD	2.78	0.46
8:1H:253:GLU:O	8:1H:257:ILE:HG12	2.16	0.46
14:1N:152:ASN:O	14:1N:156:THR:OG1	2.19	0.46
14:1N:183:SER:O	14:1N:187:MET:HG2	2.15	0.46
69:1N:401:3PE:H2F1	69:1d:201:3PE:H2I2	1.97	0.46
24:1Y:25:THR:HG23	24:1Y:67:ALA:HB2	1.98	0.46
70:1Y:202:PC1:O21	69:1m:201:3PE:H322	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1Y:207:PC1:O11	70:3T:102:PC1:H151	2.15	0.46
75:1Y:217:CDL:HB21	50:3S:19:TRP:HD1	1.80	0.46
69:1d:201:3PE:N	69:1f:101:3PE:O14	2.47	0.46
75:1d:202:CDL:H273	75:1d:202:CDL:C33	2.45	0.46
70:1h:202:PC1:H262	70:1h:202:PC1:H292	1.61	0.46
38:1m:96:PRO:HA	69:1m:205:3PE:H3H2	1.98	0.46
45:3A:49:ASN:ND2	45:3A:49:ASN:H	2.14	0.46
46:3B:95:LYS:HG2	49:3I:32:ALA:N	2.30	0.46
46:3B:290:ASN:O	46:3B:293:SER:HB3	2.16	0.46
47:3C:378:LYS:HE2	47:3C:378:LYS:HB2	1.64	0.46
49:3E:207:LYS:O	49:3E:209:GLU:N	2.49	0.46
53:3J:57:LYS:HG3	53:3J:58:HIS:N	1.95	0.46
45:3N:356:ARG:HG3	46:3O:90:GLU:O	2.15	0.46
47:3P:327:MET:HE3	70:3T:102:PC1:H3D1	1.96	0.46
51:3T:31:THR:HG23	69:3T:103:3PE:H2F1	1.96	0.46
75:3Y:106:CDL:CA6	69:3Y:107:3PE:H31	2.45	0.46
55:4A:22:PHE:HE1	91:4A:609:PGV:H151	1.80	0.46
55:4A:131:PRO:HD3	56:4B:160:LEU:HD13	1.98	0.46
55:4A:243:VAL:HG13	88:4A:602:HEA:C3C	2.45	0.46
55:4A:341:ALA:O	55:4A:345:ILE:HG13	2.16	0.46
56:4B:158:ASP:N	56:4B:158:ASP:OD1	2.49	0.46
57:4C:96:GLY:O	57:4C:99:TRP:HB3	2.15	0.46
57:4C:117:PRO:HG2	57:4C:123:PRO:HG3	1.98	0.46
57:4C:167:ILE:O	57:4C:171:VAL:HG13	2.16	0.46
57:4C:168:ALA:HB2	91:4C:302:PGV:H341	1.98	0.46
91:4C:301:PGV:H183	87:4G:103:PEK:C34	2.46	0.46
91:4C:304:PGV:H132	91:4C:304:PGV:H102	1.64	0.46
75:4C:307:CDL:H142	75:4C:307:CDL:H342	1.98	0.46
58:4D:34:SER:H	58:4D:37:GLN:HB2	1.79	0.46
1:1A:48:ARG:HD3	10:1J:76:THR:HG23	1.98	0.46
1:1A:49:LEU:H	8:1H:126:LYS:HE2	1.81	0.46
2:1B:55:CYS:HB3	2:1B:89:ALA:HB1	1.97	0.46
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.27	0.46
6:1F:92:TYR:HD1	6:1F:133:ALA:HB3	1.80	0.46
9:1I:144:HIS:CE1	16:1P:65:LEU:HD21	2.51	0.46
12:1L:257:VAL:HG23	12:1L:329:ILE:HD11	1.98	0.46
15:1O:37:ARG:O	15:1O:41:GLU:HG2	2.15	0.46
69:1Y:215:3PE:H361	69:3P:510:3PE:H281	1.97	0.46
32:1g:56:TRP:HZ2	69:1g:203:3PE:H332	1.79	0.46
45:3A:156:THR:HB	45:3A:241:ILE:CG1	2.45	0.46
46:3B:46:ARG:HG2	46:3B:379:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3B:124:LEU:HD12	46:3B:223:PHE:CB	2.34	0.46
47:3C:164:ILE:O	47:3C:177:ARG:HD2	2.15	0.46
47:3C:331:ASP:CA	47:3C:334:THR:HG22	2.43	0.46
49:3E:199:GLN:OE1	49:3E:204:ARG:HB3	2.16	0.46
49:3E:235:TYR:N	49:3E:243:TYR:HB2	2.31	0.46
50:3F:31:TRP:CE2	75:3F:201:CDL:H741	2.51	0.46
69:3G:110:3PE:H32	69:3G:111:3PE:H322	1.98	0.46
53:3J:30:LEU:HA	54:3Y:34:TRP:CD1	2.50	0.46
45:3N:70:ARG:HD3	45:3N:78:GLU:OE1	2.16	0.46
45:3N:146:ARG:O	45:3N:150:PHE:HD1	1.99	0.46
45:3N:207[B]:GLN:O	45:3N:211:LEU:HG	2.16	0.46
45:3N:445:ARG:CG	69:3N:501:3PE:H231	2.24	0.46
46:3O:314:ALA:O	46:3O:320:GLY:HA2	2.15	0.46
46:3O:370:MET:HA	46:3O:373:GLU:HG3	1.98	0.46
69:3Q:503:3PE:H2G1	69:3W:101:3PE:H3F1	1.97	0.46
49:3R:196:ARG:HE	49:3R:253:PRO:HA	1.81	0.46
49:3R:210:TRP:CZ3	49:3R:267:SER:HA	2.51	0.46
51:3T:25:ALA:C	51:3T:27:PRO:HD3	2.41	0.46
52:3U:17:LEU:HD13	52:3U:73:LEU:HD22	1.97	0.46
69:3X:101:3PE:H231	69:3X:101:3PE:C38	2.46	0.46
69:3Y:103:3PE:H372	69:3Y:105:3PE:H261	1.97	0.46
55:4A:70:VAL:O	55:4A:74:MET:HB2	2.15	0.46
55:4A:354:THR:HG23	55:4A:372:TYR:CE2	2.51	0.46
56:4B:155:SER:HB2	56:4B:179:LEU:CD1	2.46	0.46
57:4C:140:SER:CB	57:4C:242:TRP:HE1	2.29	0.46
9:1I:44:GLU:OE1	76:1I:203:AYA:C	2.64	0.46
10:1J:23:LYS:CB	11:1K:28:SER:OG	2.64	0.46
11:1K:16:LEU:O	11:1K:20:LEU:HG	2.16	0.46
12:1L:567:SER:HA	69:1L:705:3PE:H252	1.97	0.46
13:1M:29:VAL:HG21	69:1g:202:3PE:H292	1.98	0.46
77:1O:401:GTP:PA	77:1O:401:GTP:H3'	2.55	0.46
16:1P:169:SER:HB3	16:1P:231:VAL:HG23	1.97	0.46
23:1X:128:THR:HG22	27:1b:66:PRO:HG2	1.98	0.46
31:1f:25:TYR:HE1	69:1f:104:3PE:C22	2.25	0.46
38:1m:116:GLN:HB2	38:1m:117:GLU:OE1	2.15	0.46
45:3A:240:GLU:CG	51:3G:19:SER:HB2	2.46	0.46
45:3A:373:THR:HB	45:3A:374:PRO:HD3	1.98	0.46
45:3A:444:LEU:CD1	69:3A:502:3PE:H222	2.46	0.46
69:3C:506:3PE:H2I1	69:3C:507:3PE:H3H2	1.98	0.46
49:3E:265:PHE:CE2	49:3E:269:ASP:HA	2.49	0.46
69:3G:105:3PE:H122	69:3G:107:3PE:HN2	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:85:ILE:O	46:3O:89:ILE:HG13	2.16	0.46
46:3O:334:GLY:O	46:3O:338:LYS:HD3	2.15	0.46
47:3P:206:ASN:HB3	85:3P:502:HEM:O1D	2.16	0.46
48:3Q:169:LEU:HD11	48:3Q:171:PHE:CE1	2.51	0.46
69:3S:201:3PE:H2D2	69:3S:201:3PE:H2A2	1.71	0.46
54:3Y:6:LEU:HD21	69:3Y:107:3PE:C2D	2.44	0.46
54:3Y:41:ILE:HD12	69:3Y:105:3PE:C29	2.45	0.46
55:4A:367:LEU:HD21	55:4A:433:LEU:HD23	1.97	0.46
56:4B:95:LEU:HD23	56:4B:150:ILE:HG12	1.97	0.46
56:4B:112:ASP:OD1	62:4H:62:SER:HB2	2.16	0.46
57:4C:95:THR:HA	91:4C:303:PGV:H102	1.98	0.46
57:4C:109:THR:HG22	57:4C:111:GLU:H	1.81	0.46
58:4D:76:ASN:N	58:4D:76:ASN:OD1	2.48	0.46
58:4D:121:LYS:HG3	65:4K:53:TRP:HD1	1.81	0.46
59:4E:18:TYR:OH	59:4E:28:GLU:O	2.31	0.46
69:1A:201:3PE:H321	69:1b:101:3PE:C2	2.46	0.46
6:1F:367:GLU:HB2	7:1G:96:PHE:HB3	1.98	0.46
6:1F:404:ILE:HG12	71:1F:502:SF4:S1	2.56	0.46
8:1H:200:LEU:HD13	8:1H:279:ARG:HD3	1.98	0.46
12:1L:464:ALA:CA	69:1L:703:3PE:H2A2	2.46	0.46
69:1L:701:3PE:H292	69:1L:701:3PE:H262	1.75	0.46
70:1M:501:PC1:O22	70:1M:501:PC1:H31	2.17	0.46
14:1N:153:LEU:HD11	14:1N:157:MET:HE2	1.98	0.46
15:1O:296:PHE:O	15:1O:299:LEU:HB2	2.17	0.46
19:1S:68:TYR:N	19:1S:72:GLN:O	2.47	0.46
23:1X:27:ALA:O	23:1X:29:HIS:N	2.48	0.46
23:1X:46:ARG:NH1	25:1Z:80:ASP:OD2	2.49	0.46
32:1g:52:ILE:HG13	69:1g:202:3PE:H32	1.97	0.46
32:1g:64:PHE:HZ	69:1g:202:3PE:H2C2	1.81	0.46
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.34	0.46
40:1o:55:ARG:NH2	41:1p:119:SER:HB3	2.31	0.46
41:1p:25:LEU:HD23	41:1p:26:PRO:HD2	1.98	0.46
47:3C:181:PHE:CE1	47:3P:53:MET:HE2	2.51	0.46
48:3D:327:ARG:NH2	49:3E:79:SER:O	2.49	0.46
49:3E:268:ASP:O	49:3E:269:ASP:C	2.57	0.46
69:3G:107:3PE:H251	69:3G:107:3PE:H222	1.62	0.46
52:3H:93:CYS:SG	52:3H:97:LYS:HE2	2.56	0.46
45:3N:154:HIS:O	45:3N:164:ALA:HA	2.16	0.46
45:3N:173:ASN:O	45:3N:177:LEU:HG	2.16	0.46
45:3N:207[A]:GLN:O	45:3N:211:LEU:HG	2.16	0.46
46:3O:124:LEU:HD13	46:3O:223:PHE:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:184:ILE:HD11	49:3R:209:GLU:HA	1.97	0.46
49:3R:206:LYS:O	49:3R:208:PRO:HD3	2.16	0.46
69:3W:103:3PE:H2A2	69:3W:103:3PE:C36	2.46	0.46
69:4G:101:3PE:H31	69:4G:101:3PE:C22	2.44	0.46
69:1B:204:3PE:H371	75:1q:202:CDL:C59	2.44	0.45
5:1E:149:VAL:HG21	6:1F:267:THR:CG2	2.42	0.45
6:1F:57:LEU:HB3	6:1F:61:LYS:HE3	1.97	0.45
9:1I:160:LYS:HD2	9:1I:161:TRP:NE1	2.31	0.45
11:1K:73:LEU:HD23	14:1N:60:PHE:CD1	2.51	0.45
12:1L:434:LYS:HG3	36:1k:52:TYR:CD2	2.50	0.45
13:1M:401:MET:O	13:1M:405:LEU:HG	2.16	0.45
15:1O:83:TYR:OH	77:1O:401:GTP:O2'	2.34	0.45
19:1S:78:LEU:HD23	19:1S:81:PHE:CD2	2.51	0.45
20:1U:14:ARG:O	20:1U:18:VAL:HG23	2.16	0.45
69:1Y:210:3PE:H381	69:1Y:210:3PE:H352	1.47	0.45
69:1Z:201:3PE:H3B1	69:1Z:201:3PE:H382	1.60	0.45
27:1b:27:LEU:O	27:1b:31:LEU:HB2	2.16	0.45
75:1d:205:CDL:HB31	75:1d:205:CDL:HB22	1.98	0.45
32:1g:63:PHE:CE2	75:1g:201:CDL:H201	2.51	0.45
32:1g:113:PHE:O	41:1p:158:GLN:NE2	2.43	0.45
33:1h:74:TRP:HH2	69:1h:204:3PE:H2C1	1.81	0.45
33:1h:119:ASP:OD1	33:1h:119:ASP:N	2.42	0.45
39:1n:35:LYS:HE2	39:1n:35:LYS:HB3	1.72	0.45
45:3A:76:GLU:HG3	46:3B:285:VAL:HG21	1.97	0.45
45:3A:388:ARG:NH1	45:3A:390:ILE:HG12	2.31	0.45
47:3C:154:PRO:HG2	69:3C:513:3PE:H3C2	1.98	0.45
69:3C:508:3PE:H251	69:3C:508:3PE:O21	2.15	0.45
48:3D:293:MET:HE3	69:3E:303:3PE:C21	2.46	0.45
50:3F:107:LYS:CE	50:3F:111:ARG:HH12	2.29	0.45
45:3N:121:SER:CB	45:3N:123:GLU:HG2	2.45	0.45
45:3N:307:PHE:CD1	45:3N:307:PHE:C	2.93	0.45
47:3P:250:LEU:HD21	69:3P:520:3PE:H342	1.97	0.45
75:3P:513:CDL:H431	69:3P:519:3PE:H2A2	1.96	0.45
75:3P:513:CDL:H732	75:3P:513:CDL:OB8	2.16	0.45
49:3R:206:LYS:HB2	49:3R:265:PHE:CD2	2.48	0.45
52:3U:16:PRO:HG2	52:3U:77:LEU:HD21	1.98	0.45
54:3X:9:ARG:O	54:3X:13:LEU:HG	2.16	0.45
55:4A:61:HIS:HE1	88:4A:601:HEA:NB	2.14	0.45
91:4A:606:PGV:C10	58:4D:84:THR:HG22	2.46	0.45
2:1B:176:TRP:CZ2	70:1B:202:PC1:H242	2.32	0.45
70:1B:203:PC1:H2A1	70:1B:203:PC1:H271	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:39:ARG:HB2	72:1G:803:FES:S2	2.56	0.45
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.98	0.45
7:1G:254:MET:HE3	7:1G:254:MET:HB3	1.89	0.45
8:1H:173:TRP:HB2	8:1H:175:ILE:HG22	1.98	0.45
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.48	0.45
70:1H:403:PC1:C13	25:1Z:144:THR:HG22	2.46	0.45
11:1K:24:SER:O	11:1K:89:TYR:HA	2.16	0.45
12:1L:512:LYS:CG	64:4J:16:ASN:HD22	2.25	0.45
69:1L:711:3PE:H362	69:1M:502:3PE:H391	1.99	0.45
13:1M:231:LEU:HA	13:1M:235:LEU:HD12	1.97	0.45
17:1Q:37:ILE:HD12	17:1Q:103:PHE:HB2	1.97	0.45
21:1V:34:LEU:HD22	21:1V:44:ARG:HA	1.98	0.45
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.97	0.45
24:1Y:4:LEU:HA	24:1Y:7:LYS:NZ	2.31	0.45
24:1Y:112:ALA:HA	70:1Y:206:PC1:C2A	2.46	0.45
69:1Y:205:3PE:O22	69:1Y:205:3PE:H31	2.15	0.45
69:1Y:215:3PE:C2E	70:3T:102:PC1:H3A1	2.43	0.45
26:1a:6:LEU:N	26:1a:7:PRO:HD2	2.30	0.45
36:1k:13:MET:O	36:1k:13:MET:HG3	2.15	0.45
40:1o:7:ARG:NH1	40:1o:17:ASP:OD1	2.48	0.45
45:3A:124:ASP:O	45:3A:128:GLU:HG2	2.17	0.45
75:3A:501:CDL:C80	69:3Y:104:3PE:H3I2	2.46	0.45
46:3B:21:PRO:O	46:3B:22:GLN:HB2	2.16	0.45
46:3B:65:THR:HA	46:3B:186:VAL:HG11	1.98	0.45
46:3B:301:LYS:HB2	46:3B:301:LYS:NZ	2.30	0.45
47:3C:77:TRP:CZ3	48:3D:290:ARG:HG3	2.51	0.45
69:3C:509:3PE:H3E2	54:3X:32:LEU:HD23	1.98	0.45
49:3E:195:LEU:O	49:3E:196:ARG:C	2.57	0.45
75:3N:502:CDL:OB4	69:3N:503:3PE:H122	2.16	0.45
69:3N:503:3PE:C2H	70:3R:303:PC1:H2F2	2.45	0.45
69:3P:515:3PE:H2B2	69:3P:515:3PE:H2E1	1.78	0.45
69:3Q:503:3PE:H242	53:3W:47:ILE:HD11	1.98	0.45
69:3S:201:3PE:H371	69:3S:201:3PE:H342	1.65	0.45
54:3X:22:SER:OG	69:3X:106:3PE:C35	2.56	0.45
54:3Y:9:ARG:HH22	75:3Y:106:CDL:C1	2.30	0.45
54:3Y:29:ALA:HB1	69:3Y:105:3PE:H2E1	1.98	0.45
55:4A:1:FME:HCN	66:4L:12:PRO:O	2.16	0.45
55:4A:406:ASN:OD1	91:4A:606:PGV:P	2.73	0.45
75:4B:302:CDL:H151	75:4B:302:CDL:C19	2.45	0.45
1:1A:71:LEU:O	10:1J:147:TYR:OH	2.27	0.45
6:1F:189:GLU:OE1	73:1F:501:FMN:O2'	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:229:ASP:CG	7:1G:267:THR:HG23	2.41	0.45
10:1J:93:PHE:CZ	10:1J:97:LEU:HD11	2.51	0.45
10:1J:150:GLY:HA2	30:1e:16:TRP:CZ2	2.51	0.45
12:1L:203:MET:HG2	41:1p:109:LEU:HD11	1.98	0.45
12:1L:315:VAL:HG11	12:1L:412:THR:HG21	1.97	0.45
12:1L:486:MET:HA	12:1L:489:THR:HG23	1.97	0.45
69:1L:703:3PE:H332	69:1o:201:3PE:H3A2	1.98	0.45
69:1L:710:3PE:H322	69:1L:710:3PE:H351	1.57	0.45
14:1N:246:VAL:HG11	69:1N:401:3PE:H2A1	1.98	0.45
15:1O:56:ILE:O	15:1O:99:TRP:NE1	2.37	0.45
15:1O:127:SER:O	15:1O:131:ASP:HB2	2.16	0.45
16:1P:135:LEU:HD12	16:1P:167:LYS:HD3	1.98	0.45
19:1S:12:LYS:HA	19:1S:12:LYS:HD2	1.66	0.45
24:1Y:3:THR:HG23	24:1Y:4:LEU:N	2.31	0.45
24:1Y:27:ILE:CD1	69:1Y:208:3PE:H3F1	2.42	0.45
24:1Y:107:TYR:CD2	69:1Y:213:3PE:H112	2.51	0.45
28:1c:46:ASN:ND2	29:1d:20:SER:O	2.49	0.45
32:1g:63:PHE:HD2	75:1g:201:CDL:H172	1.81	0.45
34:1i:83:TYR:HD2	75:1i:201:CDL:H511	1.72	0.45
41:1p:14:ARG:HH11	41:1p:14:ARG:HG2	1.81	0.45
46:3B:25:GLU:O	46:3B:36:ALA:HA	2.15	0.45
46:3B:306:PRO:HB3	49:3I:52:ARG:N	2.31	0.45
47:3C:292:LEU:HB3	69:3C:512:3PE:H3F2	1.97	0.45
49:3E:154:ILE:HA	49:3E:274:GLY:O	2.15	0.45
49:3E:163:LYS:HB3	49:3E:165:MET:SD	2.56	0.45
50:3F:25:LEU:O	50:3F:26:GLU:C	2.57	0.45
45:3N:339:GLN:O	45:3N:343:MET:HG2	2.17	0.45
75:3N:502:CDL:H561	75:3N:502:CDL:C15	2.47	0.45
46:3O:35:ILE:HG22	46:3O:213:HIS:CE1	2.51	0.45
48:3Q:207:LYS:HA	48:3Q:210:MET:HE2	1.98	0.45
70:3R:303:PC1:H3D1	70:3R:303:PC1:H3G2	1.77	0.45
75:3X:103:CDL:H541	75:3X:103:CDL:H511	1.75	0.45
57:4C:40:MET:HE1	91:4G:102:PGV:H222	1.97	0.45
57:4C:122:HIS:CE1	61:4G:45:PRO:HB3	2.52	0.45
58:4D:67:SER:O	58:4D:71:MET:HG3	2.16	0.45
58:4D:88:PHE:HZ	67:4M:19:LEU:HD21	1.80	0.45
70:1A:202:PC1:H141	70:1P:502:PC1:H122	1.99	0.45
2:1B:71:ARG:HA	8:1H:37:PRO:HA	1.97	0.45
70:1B:203:PC1:H2	69:1B:204:3PE:C3	2.43	0.45
4:1D:259:MET:HE2	4:1D:259:MET:HB2	1.78	0.45
6:1F:110:ILE:HD12	6:1F:114:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:277:LYS:HE2	6:1F:277:LYS:HB2	1.74	0.45
69:1L:703:3PE:H252	69:1k:101:3PE:H2C2	1.98	0.45
69:1L:712:3PE:H291	37:1l:120:GLU:HG2	1.97	0.45
13:1M:190:TRP:CZ3	69:1m:201:3PE:H342	2.49	0.45
13:1M:449:LEU:HB3	70:1M:501:PC1:H32	1.98	0.45
14:1N:8:THR:CG2	75:1N:402:CDL:C40	2.94	0.45
14:1N:172:GLN:NE2	14:1N:177:LYS:HD3	2.31	0.45
15:1O:36:GLY:O	15:1O:40:ARG:HB2	2.16	0.45
15:1O:101:TYR:O	15:1O:104:ARG:HB2	2.15	0.45
15:1O:221:LEU:HD11	15:1O:241:LEU:HD11	1.98	0.45
69:1Y:213:3PE:H3D2	38:1m:94:ILE:CD1	2.46	0.45
28:1c:20:THR:O	28:1c:24:SER:OG	2.33	0.45
75:1d:205:CDL:H322	75:1d:205:CDL:HB62	1.98	0.45
34:1i:85:LEU:O	34:1i:90:THR:OG1	2.24	0.45
34:1i:89:VAL:O	34:1i:95:THR:OG1	2.32	0.45
75:3A:501:CDL:OB7	75:3A:501:CDL:H121	2.17	0.45
69:3A:502:3PE:H252	70:3J:106:PC1:O21	2.16	0.45
69:3A:503:3PE:C11	75:3Y:106:CDL:H511	2.39	0.45
49:3E:231:PHE:N	49:3E:231:PHE:CD1	2.84	0.45
49:3E:236:CYS:HB3	72:3E:301:FES:S2	2.57	0.45
45:3N:158:PHE:C	45:3N:164:ALA:HB2	2.41	0.45
45:3N:284:TYR:O	49:3V:69:GLY:O	2.35	0.45
46:3O:213:HIS:HB3	46:3O:214:PRO:HD3	1.98	0.45
47:3P:244:LEU:HA	48:3Q:201:ARG:HG3	1.97	0.45
47:3P:306:MET:CE	69:3P:514:3PE:C24	2.66	0.45
69:3P:503:3PE:O22	69:3P:505:3PE:H112	2.15	0.45
69:3P:512:3PE:H391	69:3P:512:3PE:C3D	2.38	0.45
48:3Q:75:ASN:CG	48:3Q:79:GLU:HG2	2.41	0.45
53:3W:13:LEU:HD12	69:3W:103:3PE:H292	1.98	0.45
53:3W:23:LEU:HD21	69:3X:106:3PE:H3C1	1.99	0.45
54:3Y:41:ILE:HD12	69:3Y:105:3PE:C2A	2.47	0.45
54:3Y:41:ILE:HG23	69:3Y:105:3PE:H382	1.98	0.45
54:3Y:46:PRO:O	54:3Y:49:ASN:HB2	2.16	0.45
55:4A:243:VAL:HG13	88:4A:602:HEA:C4C	2.46	0.45
91:4A:609:PGV:H21	91:4A:609:PGV:H52	1.80	0.45
93:4B:303:PSC:H02	93:4B:303:PSC:H21	1.64	0.45
57:4C:84:ILE:HG23	75:4C:306:CDL:H611	1.98	0.45
75:4C:307:CDL:C64	75:4C:307:CDL:H242	2.47	0.45
70:1A:202:PC1:H11	8:1H:62:ARG:HH22	1.82	0.45
2:1B:77:ARG:HH11	2:1B:78:ALA:H	1.63	0.45
2:1B:176:TRP:HD1	70:1B:202:PC1:O14	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:1B:203:PC1:H342	69:1B:204:3PE:H252	1.97	0.45
3:1C:188:VAL:HG12	17:1Q:78:PRO:HG3	1.98	0.45
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.56	0.45
5:1E:115:SER:HB2	5:1E:166:PRO:HG3	1.97	0.45
6:1F:98:ASP:O	73:1F:501:FMN:O4	2.34	0.45
7:1G:103:LEU:CD1	7:1G:134:LYS:HE3	2.46	0.45
8:1H:173:TRP:NE1	70:1H:404:PC1:C11	2.66	0.45
8:1H:175:ILE:C	8:1H:177:THR:N	2.74	0.45
9:1I:132:VAL:HG21	9:1I:165:ILE:HD12	1.99	0.45
76:1I:203:AYA:CB	42:1q:54:GLN:CD	2.87	0.45
10:1J:99:MET:SD	69:1J:201:3PE:C3I	3.04	0.45
12:1L:463:PHE:HB2	69:1L:703:3PE:H292	1.99	0.45
12:1L:571:MET:HE2	12:1L:571:MET:HB3	1.91	0.45
69:1L:712:3PE:H261	69:1L:712:3PE:H292	1.63	0.45
14:1N:313:MET:HG3	15:1O:270:LEU:HD13	1.98	0.45
19:1S:44:LYS:NZ	19:1S:50:LEU:O	2.42	0.45
21:1V:43:TYR:CE2	21:1V:93:MET:HG3	2.52	0.45
24:1Y:27:ILE:HD12	69:1Y:208:3PE:H3I2	1.99	0.45
24:1Y:32:GLY:HA2	24:1Y:35:VAL:HG12	1.97	0.45
29:1d:62:LEU:O	29:1d:66:THR:HG23	2.17	0.45
69:1f:104:3PE:C21	69:1f:104:3PE:H252	2.46	0.45
70:1h:203:PC1:H152	70:1h:203:PC1:O13	2.16	0.45
40:1o:19:LEU:H	40:1o:19:LEU:HD22	1.82	0.45
69:3A:502:3PE:H382	70:3J:106:PC1:C37	2.47	0.45
46:3B:47:ILE:HD11	46:3B:211:VAL:CG1	2.28	0.45
69:3C:515:3PE:H221	69:3P:514:3PE:H322	1.99	0.45
48:3D:247:ILE:HG12	48:3D:249:MET:H	1.81	0.45
49:3E:185:ASP:OD1	49:3E:186:GLN:N	2.49	0.45
49:3E:212:ILE:HG21	49:3E:273:VAL:HG21	1.98	0.45
45:3N:40:TRP:CZ2	45:3N:377:GLU:HA	2.51	0.45
45:3N:64:PHE:HZ	45:3N:88:ALA:HB2	1.81	0.45
45:3N:431:LEU:HD12	45:3N:432:PRO:HD2	1.97	0.45
47:3P:67:THR:HG22	48:3Q:115:TYR:HE2	1.81	0.45
48:3Q:105:ASN:HD21	48:3Q:110:PRO:CG	2.29	0.45
48:3Q:208:MET:HA	69:3R:302:3PE:H321	1.99	0.45
49:3R:93:ARG:HB3	69:3R:305:3PE:H112	1.97	0.45
69:3T:103:3PE:H2E1	69:3T:103:3PE:H2H2	1.58	0.45
55:4A:274:VAL:HA	55:4A:277:MET:HE2	1.99	0.45
55:4A:468:MET:HA	55:4A:468:MET:HE3	1.98	0.45
75:4B:302:CDL:H541	75:4B:302:CDL:H111	1.99	0.45
62:4H:33:TYR:OH	62:4H:73:ASP:OD1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:18:VAL:HA	1:1A:21:ALA:HB3	1.97	0.45
69:1A:201:3PE:H2E1	69:1A:201:3PE:H2B2	1.66	0.45
69:1A:203:3PE:C23	14:1N:2:ASN:HD21	2.30	0.45
4:1D:237:ASN:HB3	8:1H:284:GLN:NE2	2.32	0.45
7:1G:43:HIS:CD2	7:1G:45:ARG:H	2.34	0.45
7:1G:172:LEU:HD23	7:1G:199:ILE:HD13	1.97	0.45
13:1M:104:LEU:HD12	13:1M:107:ILE:HD11	1.98	0.45
15:1O:36:GLY:C	15:1O:40:ARG:HH12	2.25	0.45
15:1O:97:GLN:HG2	15:1O:135:LEU:HD12	1.98	0.45
21:1V:13:LEU:HD23	21:1V:13:LEU:HA	1.80	0.45
24:1Y:31:THR:CG2	69:1Y:208:3PE:H2C1	2.47	0.45
24:1Y:75:ILE:HG21	69:1Y:201:3PE:H282	1.98	0.45
29:1d:53:VAL:HG21	69:1d:201:3PE:H221	1.99	0.45
75:1d:205:CDL:H351	75:1d:205:CDL:C12	2.42	0.45
75:1g:201:CDL:HA4	33:1h:27:PHE:CE2	2.51	0.45
33:1h:75:ILE:HG23	33:1h:79:PHE:HE1	1.82	0.45
40:1o:62:LEU:HD23	40:1o:86:TRP:CZ2	2.52	0.45
45:3A:158:PHE:HB3	45:3A:161:THR:OG1	2.16	0.45
46:3B:424:MET:HB3	46:3B:436:VAL:HG22	1.99	0.45
48:3D:240:TYR:OH	52:3H:91:ASP:OD2	2.31	0.45
49:3E:211:VAL:HG21	49:3E:246:SER:O	2.15	0.45
69:3J:103:3PE:H241	69:3J:103:3PE:H272	1.81	0.45
45:3N:280:TYR:HA	45:3N:284:TYR:CE2	2.52	0.45
47:3P:109:PHE:HB3	47:3P:112:THR:CG2	2.47	0.45
47:3P:112:THR:O	47:3P:196:HIS:CE1	2.69	0.45
47:3P:295:VAL:HG23	69:3P:518:3PE:H3F1	1.98	0.45
69:3P:507:3PE:O22	69:3P:507:3PE:H352	2.15	0.45
75:3P:513:CDL:H522	75:3P:513:CDL:HA32	1.97	0.45
69:3P:515:3PE:H2D1	69:3P:516:3PE:H2E2	1.98	0.45
69:3Q:502:3PE:H332	69:3Q:502:3PE:H2	1.99	0.45
49:3R:159:ILE:HA	49:3R:165:MET:CG	2.47	0.45
49:3R:169:TRP:CD1	49:3R:174:LEU:HD22	2.51	0.45
49:3R:192:VAL:HG13	49:3R:199:GLN:H	1.82	0.45
49:3R:231:PHE:CE1	49:3R:251:LYS:HE2	2.52	0.45
69:3R:302:3PE:H2B1	69:3R:302:3PE:H3G1	1.97	0.45
69:3X:108:3PE:H332	69:4G:104:3PE:C35	2.38	0.45
55:4A:202:LEU:O	55:4A:206:ILE:HG12	2.16	0.45
55:4A:278:MET:CE	91:4A:607:PGV:H51	2.47	0.45
68:4N:27:THR:O	68:4N:28:GLY:C	2.59	0.45
1:1A:107:THR:OG1	69:1A:203:3PE:H332	2.16	0.45
2:1B:58:GLU:HG2	2:1B:151:PRO:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:41:GLY:O	44:1s:73:PRO:HD3	2.16	0.45
7:1G:237:ASN:HB3	7:1G:253:ARG:HE	1.82	0.45
7:1G:444:LYS:NZ	7:1G:480:SER:HB2	2.32	0.45
8:1H:92:PRO:HD3	8:1H:255:TYR:CD1	2.52	0.45
11:1K:59:MET:HE2	14:1N:84:TRP:CH2	2.50	0.45
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.98	0.45
75:1L:704:CDL:H761	13:1M:369:LEU:HD21	1.98	0.45
13:1M:127:VAL:CB	69:1N:401:3PE:H3H1	2.47	0.45
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	1.99	0.45
24:1Y:134:VAL:CG2	69:1Y:211:3PE:H262	2.46	0.45
69:1Y:215:3PE:H3C1	69:3P:510:3PE:H2I1	1.98	0.45
69:1d:203:3PE:H2D1	69:1d:203:3PE:H2G2	1.34	0.45
31:1f:22:PHE:CE1	69:1f:104:3PE:H321	2.52	0.45
32:1g:64:PHE:CZ	69:1g:202:3PE:H2C2	2.51	0.45
69:1m:202:3PE:H231	69:1m:202:3PE:H2	1.99	0.45
69:1m:204:3PE:H231	69:1m:204:3PE:H2I3	1.98	0.45
39:1n:97:LYS:HD2	39:1n:173:PRO:HB2	1.99	0.45
69:3A:503:3PE:H252	69:3A:503:3PE:H221	1.79	0.45
47:3C:101:GLY:HA2	47:3C:106:SER:HB2	1.98	0.45
49:3E:223:VAL:HG21	48:3Q:144:ARG:HH22	1.82	0.45
69:3G:101:3PE:H241	69:3G:101:3PE:H271	1.67	0.45
69:3G:111:3PE:H372	69:3G:111:3PE:H3A1	1.78	0.45
46:3O:192:HIS:O	46:3O:196:GLN:HG3	2.16	0.45
47:3P:19:ILE:HG23	47:3P:221:HIS:HB2	1.99	0.45
47:3P:141:TRP:CE3	47:3P:264:THR:HG23	2.51	0.45
75:3P:513:CDL:H341	75:3P:513:CDL:H152	1.98	0.45
49:3R:149:MET:C	49:3R:151:LYS:N	2.69	0.45
49:3R:179:ARG:HD2	49:3R:211:VAL:HB	1.98	0.45
49:3R:219:HIS:CB	72:3R:301:FES:S2	3.05	0.45
69:3S:201:3PE:H3A1	69:3S:201:3PE:H2F2	1.99	0.45
52:3U:28:GLU:C	52:3U:32:LYS:HZ3	2.24	0.45
54:3X:44:TRP:CG	69:3X:108:3PE:H381	2.50	0.45
55:4A:507:GLU:OE2	60:4F:51:SER:HA	2.16	0.45
64:4J:41:GLY:CA	91:4J:101:PGV:H292	2.47	0.45
1:1A:41:PHE:CZ	2:1B:99:ALA:HB2	2.52	0.45
1:1A:106:TRP:CZ3	69:1A:201:3PE:H251	2.51	0.45
4:1D:208:LEU:HD22	4:1D:315:LEU:HD23	1.99	0.45
4:1D:234:ILE:O	4:1D:238:ARG:HG3	2.16	0.45
4:1D:339:LYS:HE2	9:1I:127:PRO:O	2.17	0.45
7:1G:40:PHE:O	7:1G:158:ARG:NE	2.39	0.45
7:1G:443:LEU:HD12	7:1G:477:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:260:VAL:HA	8:1H:263:THR:HG22	1.99	0.45
9:1I:66:ALA:HB1	9:1I:158:GLY:HA2	1.98	0.45
12:1L:464:ALA:HB2	69:1L:703:3PE:C2A	2.42	0.45
12:1L:524:ASN:ND2	39:1n:77:GLN:HG2	2.18	0.45
12:1L:538:THR:OG1	69:1L:701:3PE:H241	2.17	0.45
75:1L:704:CDL:H521	75:1L:704:CDL:H372	1.99	0.45
69:1L:710:3PE:C22	33:1h:26:ARG:HD3	2.46	0.45
14:1N:98:MET:HA	14:1N:101:ALA:HB3	1.98	0.45
14:1N:220:ILE:HG22	14:1N:323:MET:HE1	1.98	0.45
14:1N:245:MET:HE1	69:1N:401:3PE:H3B1	1.98	0.45
15:1O:315:LYS:HA	15:1O:315:LYS:HD2	1.71	0.45
16:1P:167:LYS:HG3	16:1P:229:ALA:HA	1.99	0.45
69:1f:102:3PE:H322	69:1g:203:3PE:H391	1.99	0.45
32:1g:87:GLU:O	32:1g:91:ARG:HG3	2.17	0.45
69:1l:204:3PE:H352	69:1l:204:3PE:C31	2.47	0.45
46:3B:95:LYS:HZ1	49:3I:69:GLY:HA3	1.82	0.45
69:3C:511:3PE:C39	69:3C:512:3PE:H2B1	2.41	0.45
48:3D:99:PRO:HD3	52:3H:95:ALA:O	2.17	0.45
53:3J:15:PHE:CD1	53:3J:21:PHE:HD1	2.34	0.45
45:3N:366:VAL:HG22	45:3N:392:LEU:HD13	1.99	0.45
69:3P:507:3PE:C2A	69:3P:507:3PE:H3C1	2.47	0.45
75:3P:513:CDL:C20	69:3P:520:3PE:H2D1	2.44	0.45
49:3R:179:ARG:HD2	49:3R:211:VAL:N	2.31	0.45
69:3W:103:3PE:H2	69:3W:103:3PE:C11	2.47	0.45
69:3Y:105:3PE:H382	69:3Y:105:3PE:H3B1	1.62	0.45
55:4A:22:PHE:HB2	91:4A:609:PGV:H11	1.99	0.45
55:4A:230:LEU:HB2	57:4C:103:HIS:CE1	2.51	0.45
55:4A:409:TRP:NE1	91:4A:606:PGV:H31	2.30	0.45
57:4C:187:THR:HA	87:4G:103:PEK:H041	1.98	0.45
58:4D:83:GLY:HA3	65:4K:17:ILE:HG22	1.99	0.45
1:1A:104:TYR:HB2	69:1A:203:3PE:H372	1.99	0.45
8:1H:93:TYR:OH	26:1a:35:GLU:OE2	2.29	0.45
8:1H:111:LEU:HD11	10:1J:57:PHE:CE1	2.52	0.45
10:1J:14:VAL:HG11	11:1K:10:MET:HG2	1.98	0.45
10:1J:88:THR:HB	11:1K:23:ARG:HH21	1.82	0.45
10:1J:96:GLY:HA3	69:1J:203:3PE:C39	2.46	0.45
11:1K:40:LEU:HD13	14:1N:71:MET:HB3	1.99	0.45
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.99	0.45
69:1L:703:3PE:H242	69:1L:703:3PE:H271	1.53	0.45
13:1M:366:ASN:ND2	13:1M:407:SER:OG	2.37	0.45
14:1N:193:VAL:HG23	14:1N:269:GLU:CD	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:80:GLU:HB3	15:1O:190:HIS:CE1	2.52	0.45
15:1O:100:LEU:C	15:1O:100:LEU:HD12	2.42	0.45
15:1O:105:LEU:HD21	15:1O:159:THR:HB	1.99	0.45
24:1Y:4:LEU:O	24:1Y:7:LYS:CG	2.65	0.45
69:1Y:215:3PE:H292	69:1Y:216:3PE:H291	1.98	0.45
40:1o:15:GLU:HG3	40:1o:105:ARG:HD2	1.99	0.45
69:1o:201:3PE:O14	41:1p:23:THR:HG22	2.16	0.45
45:3A:79:VAL:HG21	45:3A:86:LEU:HD12	1.99	0.45
45:3A:230:ALA:O	45:3A:231:PHE:HB3	2.17	0.45
45:3A:244:ARG:HD3	51:3G:12:MET:CE	2.47	0.45
45:3A:442:PHE:CE1	69:3A:502:3PE:H121	2.51	0.45
69:3A:503:3PE:H2C1	69:3A:503:3PE:H292	1.70	0.45
46:3B:253:VAL:HG11	46:3B:433:THR:OG1	2.17	0.45
46:3B:309:VAL:HG21	46:3B:340:ALA:HB2	1.98	0.45
48:3D:245:GLN:HG2	52:3H:84:PHE:CZ	2.45	0.45
45:3N:214:LYS:HE2	45:3N:214:LYS:HB2	1.78	0.45
46:3O:56:ARG:NH1	46:3O:103:GLU:OE2	2.50	0.45
69:3P:507:3PE:C22	54:3Y:38:TRP:CG	2.99	0.45
49:3R:200:HIS:CD2	49:3R:202:LEU:HB2	2.52	0.45
75:3X:103:CDL:H821	75:3X:103:CDL:H792	1.78	0.45
69:3X:107:3PE:H291	69:4G:101:3PE:H261	1.99	0.45
68:4N:32:TYR:C	68:4N:34:THR:N	2.75	0.45
1:1A:25:PRO:HB3	8:1H:58:LYS:O	2.16	0.45
1:1A:108:GLN:HE21	69:1A:203:3PE:C24	2.29	0.45
3:1C:179:GLU:OE1	16:1P:37:HIS:NE2	2.50	0.45
4:1D:19:MET:HE2	4:1D:19:MET:HB2	1.88	0.45
4:1D:230:THR:O	4:1D:294:TYR:OH	2.22	0.45
4:1D:338:MET:HE2	4:1D:348:HIS:CE1	2.52	0.45
6:1F:250:ASN:O	6:1F:250:ASN:ND2	2.38	0.45
8:1H:121:TRP:HZ2	10:1J:80:PRO:HB2	1.82	0.45
75:1H:401:CDL:H511	75:1H:401:CDL:HB4	1.86	0.45
10:1J:125:TRP:HH2	25:1Z:126:GLY:HA2	1.81	0.45
12:1L:16:THR:O	12:1L:20:MET:HG3	2.17	0.45
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.82	0.45
70:1Y:206:PC1:C28	70:1Y:207:PC1:H2E1	2.47	0.45
75:1Y:217:CDL:H211	75:1Y:217:CDL:H391	1.99	0.45
32:1g:77:VAL:HA	32:1g:80:LEU:HG	1.99	0.45
45:3A:12:PRO:HG2	45:3A:28:GLU:OE2	2.18	0.45
45:3A:411:CYS:O	45:3A:415:PHE:HB2	2.17	0.45
47:3C:334:THR:HG21	69:3G:111:3PE:H3C2	1.99	0.45
69:3C:513:3PE:O21	69:3C:513:3PE:H242	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3D:238:ASN:O	48:3D:245:GLN:HA	2.17	0.45
48:3D:314:HIS:O	51:3G:22:PRO:HB3	2.17	0.45
49:3E:249:ILE:HG22	49:3E:257:ASN:HB3	1.97	0.45
69:3G:106:3PE:H222	69:3G:106:3PE:H2	1.68	0.45
45:3N:64:PHE:CZ	45:3N:88:ALA:HB2	2.51	0.45
69:3P:503:3PE:H3G2	69:3P:503:3PE:H3D1	1.67	0.45
49:3R:187:GLU:HG3	49:3R:244:ASP:CG	2.42	0.45
54:3X:39:ARG:HE	54:3X:39:ARG:HB3	1.53	0.45
54:3Y:39:ARG:HG2	54:3Y:52:PHE:CZ	2.51	0.45
55:4A:172:LYS:HG3	55:4A:173:PRO:HD2	1.99	0.45
55:4A:484:ALA:HB3	67:4M:2:TYR:HB2	1.98	0.45
61:4G:76:ASN:OD1	87:4G:103:PEK:N	2.50	0.45
64:4J:55:PHE:HB2	64:4J:57:HIS:CE1	2.52	0.45
1:1A:23:TRP:CG	70:1A:202:PC1:O12	2.69	0.44
69:1B:204:3PE:H2F2	69:1B:204:3PE:H2I3	1.80	0.44
3:1C:45:PHE:HD1	3:1C:47:GLU:HG3	1.82	0.44
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.99	0.44
6:1F:252:GLY:O	6:1F:272:MET:HB3	2.17	0.44
10:1J:79:TYR:HB2	16:1P:325:ARG:NH1	2.32	0.44
69:1J:203:3PE:H3C2	69:1J:203:3PE:H392	1.76	0.44
13:1M:22:MET:HE3	13:1M:22:MET:HB3	1.92	0.44
14:1N:245:MET:HB2	14:1N:301:SER:OG	2.17	0.44
75:1N:402:CDL:H161	69:1e:201:3PE:H322	1.99	0.44
75:1N:402:CDL:H532	69:1e:201:3PE:O32	2.16	0.44
15:1O:318:TRP:HB2	29:1d:58:LEU:HD12	1.98	0.44
16:1P:83:LYS:HB3	16:1P:83:LYS:HE2	1.79	0.44
20:1T:36:PHE:HA	20:1T:40:LEU:HD12	1.99	0.44
69:1Y:213:3PE:H2G1	69:1Y:213:3PE:H2D1	1.67	0.44
26:1a:49:GLU:OE2	26:1a:52:ARG:NH2	2.37	0.44
31:1f:25:TYR:O	31:1f:29:ARG:HG2	2.17	0.44
75:1g:201:CDL:H791	33:1h:35:PRO:CG	2.39	0.44
33:1h:77:ARG:HE	69:1h:204:3PE:C3	2.30	0.44
42:1q:1:MET:HG3	42:1q:2:GLU:N	2.32	0.44
47:3C:264:THR:OG1	47:3C:268:ILE:HD11	2.16	0.44
47:3C:331:ASP:C	47:3C:334:THR:HG22	2.42	0.44
69:3C:507:3PE:C29	69:3C:508:3PE:H281	2.46	0.44
69:3C:515:3PE:H11	69:3C:516:3PE:C1	2.47	0.44
48:3D:305:LEU:HB3	69:3G:101:3PE:C3B	2.46	0.44
49:3E:228:ALA:N	49:3E:233:GLY:O	2.51	0.44
75:3F:201:CDL:H361	69:3G:109:3PE:H232	1.99	0.44
75:3N:502:CDL:H651	69:3R:304:3PE:H3I2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3P:515:3PE:H3I3	69:3P:517:3PE:H2B1	1.98	0.44
69:3P:519:3PE:H272	69:3P:519:3PE:C35	2.45	0.44
48:3Q:144:ARG:CG	48:3Q:147:LEU:HD22	2.38	0.44
49:3R:179:ARG:HB2	49:3R:184:ILE:HG12	1.99	0.44
51:3T:51:PRO:HD3	70:3T:102:PC1:H372	1.99	0.44
69:3W:101:3PE:H271	69:3W:101:3PE:H2A2	1.73	0.44
69:3Y:102:3PE:H31	69:3Y:102:3PE:P	2.57	0.44
91:4A:607:PGV:H42	75:4C:306:CDL:H431	1.99	0.44
91:4G:102:PGV:H291	91:4G:102:PGV:H262	1.72	0.44
1:1A:42:ASP:OD1	1:1A:42:ASP:N	2.40	0.44
2:1B:92:LEU:HB3	2:1B:133:VAL:CG1	2.47	0.44
4:1D:49:LEU:HD12	4:1D:49:LEU:HA	1.82	0.44
4:1D:50:ASN:HA	4:1D:65:VAL:HA	1.97	0.44
6:1F:84:LYS:HB2	6:1F:84:LYS:HE3	1.63	0.44
6:1F:362:CYS:HB3	6:1F:404:ILE:CG2	2.47	0.44
7:1G:356:THR:HG22	7:1G:503:LEU:HG	1.99	0.44
7:1G:444:LYS:HA	7:1G:444:LYS:HD2	1.84	0.44
8:1H:179:TRP:CE2	8:1H:180:PRO:HD3	2.52	0.44
8:1H:215:TYR:HD1	8:1H:219:PRO:HB2	1.82	0.44
70:1H:403:PC1:H133	70:1H:403:PC1:O12	2.17	0.44
12:1L:548:SER:HA	12:1L:552:LEU:HB3	1.99	0.44
12:1L:556:ILE:HD13	38:1m:79:PHE:HB2	2.00	0.44
14:1N:40:MET:O	14:1N:43:VAL:HG22	2.17	0.44
16:1P:69:ILE:HD12	18:1R:26:VAL:HG13	1.98	0.44
16:1P:100:GLU:OE2	16:1P:144:ARG:NH1	2.51	0.44
19:1S:50:LEU:HD22	19:1S:94:LEU:HD21	2.00	0.44
70:1Y:202:PC1:H241	69:1m:201:3PE:H331	1.98	0.44
30:1e:64:GLU:O	30:1e:68:ARG:HD2	2.16	0.44
32:1g:45:HIS:HB2	32:1g:54:ASP:OD1	2.18	0.44
45:3A:394:GLU:HG2	45:3A:398:ARG:HE	1.82	0.44
47:3C:51:LEU:HD13	85:3C:501:HEM:HBD1	1.99	0.44
69:3C:512:3PE:N	69:3C:512:3PE:H11	2.32	0.44
51:3G:21:SER:HB3	51:3G:24:GLU:HG2	1.99	0.44
52:3H:41:PRO:HG2	52:3H:102:LEU:HD23	1.99	0.44
69:3J:105:3PE:H2	54:3Y:47:TYR:CD1	2.53	0.44
69:3N:501:3PE:H3A2	69:3N:501:3PE:H3D1	1.84	0.44
75:3N:502:CDL:C86	54:3X:25:GLY:HA2	2.47	0.44
75:3P:513:CDL:OA9	75:3P:513:CDL:HA4	2.18	0.44
69:3Q:504:3PE:H342	69:3Q:504:3PE:H382	1.98	0.44
50:3S:105:GLU:HG2	54:3Y:4:ARG:HG3	1.99	0.44
52:3U:22:GLU:HA	52:3U:25:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:3U:42:GLN:H	52:3U:42:GLN:HG2	1.51	0.44
69:3W:103:3PE:H382	54:3X:23:MET:CE	2.45	0.44
55:4A:8:TYR:O	57:4C:13:PRO:HB3	2.17	0.44
55:4A:208:MET:HE1	55:4A:234:LEU:CD1	2.47	0.44
55:4A:353:LEU:O	55:4A:357:VAL:HG13	2.17	0.44
75:4B:302:CDL:H152	75:4B:302:CDL:H471	2.00	0.44
91:4N:101:PGV:H161	91:4N:101:PGV:C12	2.44	0.44
4:1D:18:VAL:HG22	4:1D:20:TYR:H	1.82	0.44
10:1J:41:CYS:O	10:1J:45:LEU:HG	2.17	0.44
11:1K:2:PRO:HB3	30:1e:72:MET:HE1	1.99	0.44
12:1L:88:MET:HE2	12:1L:88:MET:HB2	1.77	0.44
18:1R:74:ASN:OD1	18:1R:76:ASP:HB2	2.18	0.44
32:1g:76:PHE:HB2	70:1h:203:PC1:H372	2.00	0.44
69:1m:205:3PE:H2I2	69:1m:205:3PE:H2F2	1.81	0.44
39:1n:91:GLU:HB2	39:1n:94:GLU:HG3	1.99	0.44
45:3A:106:LEU:HB3	45:3A:107:PRO:HD3	1.99	0.44
45:3A:439:SER:HA	45:3A:442:PHE:CE2	2.52	0.44
46:3B:149:ALA:O	46:3B:153:GLN:HG3	2.17	0.44
46:3B:182:ARG:NH2	46:3B:186:VAL:HG22	2.31	0.44
47:3C:291:VAL:O	47:3C:295:VAL:HG22	2.17	0.44
69:3C:513:3PE:H242	69:3C:513:3PE:H351	1.98	0.44
52:3H:50:GLU:HG2	52:3H:86:PHE:CZ	2.52	0.44
46:3O:31:ASN:OD1	46:3O:31:ASN:N	2.51	0.44
46:3O:272:PHE:HZ	46:3O:416:LYS:HD2	1.81	0.44
47:3P:116:GLY:C	85:3P:502:HEM:HBC2	2.41	0.44
47:3P:253:PRO:HG3	69:3P:520:3PE:H122	1.99	0.44
69:3P:507:3PE:O21	54:3Y:38:TRP:CD1	2.70	0.44
51:3T:67:GLU:HA	51:3T:70:LYS:HE3	1.98	0.44
55:4A:295:VAL:CG2	55:4A:297:MET:HG3	2.48	0.44
56:4B:110:TYR:HB2	56:4B:116:LEU:HB3	1.98	0.44
57:4C:156:ARG:NH2	57:4C:222:GLN:O	2.50	0.44
65:4K:16:ALA:O	65:4K:20:SER:OG	2.30	0.44
1:1A:26:GLN:O	1:1A:27:LEU:HD12	2.17	0.44
1:1A:39:CYS:O	4:1D:53:PRO:HD2	2.18	0.44
4:1D:90:LEU:O	4:1D:94:LYS:HG3	2.18	0.44
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.98	0.44
6:1F:353:PHE:O	6:1F:357:GLU:HG2	2.18	0.44
8:1H:181:LEU:HD12	8:1H:304:HIS:CE1	2.51	0.44
70:1H:402:PC1:H153	70:1H:402:PC1:O13	2.18	0.44
70:1H:403:PC1:H2F2	10:1J:39:VAL:CG1	2.47	0.44
12:1L:517:SER:OG	69:1L:708:3PE:O13	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:149:PHE:O	13:1M:153:THR:HG23	2.18	0.44
14:1N:135:LYS:HD2	14:1N:187:MET:SD	2.58	0.44
15:1O:104:ARG:O	15:1O:107:GLN:N	2.50	0.44
18:1R:52:VAL:HG21	18:1R:57:ILE:HG12	2.00	0.44
19:1S:78:LEU:HD22	19:1S:86:VAL:HG13	1.99	0.44
24:1Y:5:LEU:HD22	69:1Y:211:3PE:O32	2.15	0.44
24:1Y:78:GLN:CD	51:3T:56:TYR:HH	2.25	0.44
24:1Y:79:VAL:HG12	69:1Y:214:3PE:O13	2.17	0.44
82:1Y:203:PGT:H132	82:1Y:203:PGT:H171	1.99	0.44
69:1Y:213:3PE:H372	69:1Y:213:3PE:H2D2	1.99	0.44
25:1Z:8:GLN:HG2	43:1r:40:LEU:HD23	1.99	0.44
69:1d:203:3PE:H351	69:1d:203:3PE:H321	1.86	0.44
34:1i:92:LYS:HB2	34:1i:92:LYS:HE2	1.81	0.44
69:1l:204:3PE:H261	69:1l:204:3PE:H291	1.69	0.44
39:1n:30:CYS:O	39:1n:32:HIS:N	2.48	0.44
45:3A:155:ALA:HA	45:3A:164:ALA:HB1	1.99	0.44
45:3A:192:ALA:N	45:3A:220:SER:OG	2.45	0.44
46:3B:163:LEU:HD11	46:3B:258:VAL:HG22	1.99	0.44
45:3N:86:LEU:HD13	45:3N:99:ILE:CG1	2.46	0.44
75:3N:502:CDL:H361	75:3N:502:CDL:H212	1.98	0.44
48:3Q:225:HIS:O	51:3T:20:PRO:HB3	2.18	0.44
49:3R:131:ASN:OD1	69:3R:302:3PE:H112	2.17	0.44
69:3R:302:3PE:H3E1	69:3R:302:3PE:H3H2	1.74	0.44
69:3R:304:3PE:H2B1	69:3R:304:3PE:H282	1.85	0.44
69:3W:101:3PE:H11	69:3W:101:3PE:C12	2.48	0.44
69:3X:106:3PE:H3D2	69:3X:106:3PE:H3A2	1.84	0.44
54:3Y:44:TRP:HB2	69:3Y:105:3PE:H3A2	1.99	0.44
69:3Y:102:3PE:H3G1	69:3Y:105:3PE:H3I2	2.00	0.44
69:3Y:104:3PE:H3I3	69:3Y:104:3PE:H3F1	1.77	0.44
55:4A:346:PHE:CD2	91:4A:608:PGV:H281	2.52	0.44
56:4B:29:MET:HE3	56:4B:29:MET:HB3	1.73	0.44
91:4C:302:PGV:H271	91:4C:302:PGV:H11	1.99	0.44
68:4N:20:VAL:O	68:4N:24:ALA:N	2.51	0.44
68:4N:62:GLN:NE2	68:4N:64:LYS:O	2.49	0.44
4:1D:245:VAL:HG21	4:1D:255:PHE:HE2	1.82	0.44
5:1E:214:GLN:H	5:1E:217:LEU:HB3	1.82	0.44
8:1H:86:TRP:NE1	8:1H:233:MET:HB2	2.33	0.44
8:1H:243:LEU:O	8:1H:262:LYS:HE3	2.17	0.44
10:1J:17:PHE:HB3	11:1K:14:ILE:HG12	1.98	0.44
13:1M:66:LEU:HD11	13:1M:111:THR:HG23	1.99	0.44
14:1N:128:LEU:HD12	14:1N:216:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:245:MET:SD	14:1N:249:LEU:HD11	2.57	0.44
69:1N:401:3PE:H3I3	69:1N:401:3PE:H3F1	1.60	0.44
16:1P:168:PRO:HA	16:1P:230:PHE:O	2.17	0.44
22:1W:86:GLY:HA2	22:1W:89:GLU:OE1	2.16	0.44
69:1Y:215:3PE:H3C1	69:3P:510:3PE:C2I	2.48	0.44
25:1Z:57:ARG:HA	25:1Z:60:LEU:HD12	1.99	0.44
29:1d:27:THR:HG21	69:1f:104:3PE:P	2.57	0.44
69:1d:206:3PE:H382	69:1f:104:3PE:H342	1.99	0.44
33:1h:24:LEU:HD12	33:1h:24:LEU:HA	1.87	0.44
39:1n:80:ILE:H	39:1n:80:ILE:HD12	1.81	0.44
45:3A:77:LYS:HE3	45:3A:77:LYS:HB2	1.70	0.44
46:3B:378:PHE:O	46:3B:382:VAL:HG23	2.18	0.44
47:3C:36:LEU:HB3	47:3C:235:MET:SD	2.58	0.44
47:3C:307:LEU:O	47:3C:309:THR:HG23	2.17	0.44
48:3D:286:GLU:OE1	48:3D:286:GLU:N	2.51	0.44
69:3D:503:3PE:H371	69:3D:503:3PE:H3A1	1.87	0.44
50:3F:63:PRO:HD3	50:3F:105:TYR:CZ	2.52	0.44
69:3G:107:3PE:H351	69:3G:107:3PE:H322	1.77	0.44
45:3N:403:ASP:OD1	45:3N:406:VAL:HG23	2.17	0.44
75:3N:502:CDL:H311	47:3P:19:ILE:CD1	2.48	0.44
46:3O:168:TYR:N	46:3O:240:ARG:HG2	2.32	0.44
49:3R:153:GLU:O	49:3R:155:LYS:NZ	2.51	0.44
54:3X:44:TRP:NE1	69:3X:108:3PE:H221	2.32	0.44
75:3Y:106:CDL:HA62	69:3Y:107:3PE:O32	2.16	0.44
55:4A:54:TYR:O	55:4A:58:VAL:HG23	2.17	0.44
60:4F:10:GLU:HA	60:4F:21:MET:HE1	1.98	0.44
4:1D:14:PHE:HD1	4:1D:19:MET:SD	2.40	0.44
4:1D:121:ALA:HA	4:1D:365:THR:HG21	2.00	0.44
5:1E:106:THR:HB	5:1E:107:PRO:HD3	1.99	0.44
5:1E:172:ILE:HG12	5:1E:187:ARG:HH21	1.82	0.44
7:1G:195:LEU:HB3	7:1G:198:ASN:HD22	1.82	0.44
8:1H:187:ILE:CG1	70:1H:402:PC1:H251	2.48	0.44
70:1J:202:PC1:H371	70:1J:202:PC1:H342	1.54	0.44
69:1L:706:3PE:H372	69:1Y:204:3PE:H251	2.00	0.44
13:1M:8:THR:HG21	13:1M:103:GLN:HG2	1.99	0.44
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.18	0.44
15:1O:291:ARG:NE	32:1g:29:ASP:OD2	2.38	0.44
16:1P:169:SER:OG	16:1P:203:GLN:O	2.33	0.44
16:1P:274:PRO:HD2	16:1P:275:PHE:CE2	2.53	0.44
20:1T:16:LEU:O	20:1T:20:LYS:HG3	2.17	0.44
24:1Y:62:SER:HB3	69:1Y:208:3PE:C38	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
82:1Y:203:PGT:H211	82:1Y:203:PGT:H182	1.86	0.44
32:1g:26:LEU:HD12	32:1g:26:LEU:HA	1.75	0.44
69:1g:202:3PE:H2G1	69:1g:202:3PE:H2D1	1.67	0.44
33:1h:50:ALA:HB2	41:1p:60:TYR:CE1	2.53	0.44
34:1i:83:TYR:CE2	75:1i:201:CDL:C51	2.90	0.44
46:3B:308:ASP:HB3	46:3B:327:ILE:HB	2.00	0.44
47:3C:4:ILE:CG1	47:3C:8:HIS:HB2	2.45	0.44
48:3D:253:ILE:HG22	48:3D:254:TYR:N	2.33	0.44
69:3E:302:3PE:H251	69:3E:302:3PE:H281	1.54	0.44
75:3F:201:CDL:C27	69:3G:109:3PE:H3G1	2.48	0.44
51:3G:38:ASN:O	51:3G:42:ARG:HG3	2.18	0.44
45:3N:358:LYS:HE3	45:3N:399:ILE:O	2.18	0.44
46:3O:28:ARG:NH2	46:3O:32:GLY:O	2.51	0.44
46:3O:342:ASP:O	46:3O:346:THR:HG23	2.18	0.44
47:3P:270:PRO:HG2	47:3P:275:LEU:HD23	1.98	0.44
69:3P:503:3PE:H382	69:3P:505:3PE:H351	1.96	0.44
69:3P:503:3PE:H321	69:3P:504:3PE:P	2.57	0.44
49:3R:179:ARG:H	49:3R:179:ARG:HG3	1.61	0.44
49:3R:243:TYR:HA	49:3R:248:ARG:O	2.18	0.44
69:3W:102:3PE:H382	69:3W:102:3PE:C25	2.34	0.44
55:4A:25:TRP:CB	91:4A:609:PGV:H291	2.41	0.44
55:4A:208:MET:HE1	55:4A:234:LEU:HD11	1.99	0.44
59:4E:16:VAL:O	59:4E:16:VAL:HG12	2.17	0.44
62:4H:31:GLN:NE2	62:4H:35:ASP:OD2	2.45	0.44
4:1D:234:ILE:HD12	8:1H:277:TYR:HB3	1.98	0.44
4:1D:342:MET:HA	4:1D:342:MET:HE2	2.00	0.44
6:1F:109:GLU:O	6:1F:113:HIS:HB2	2.18	0.44
13:1M:410:MET:O	13:1M:414:THR:OG1	2.24	0.44
15:1O:28:ASP:HB2	15:1O:171:TYR:HD1	1.83	0.44
15:1O:100:LEU:HD21	77:1O:401:GTP:N1	2.32	0.44
77:1O:401:GTP:H3'	77:1O:401:GTP:O2A	2.17	0.44
17:1Q:75:THR:OG1	17:1Q:77:ASP:OD1	2.35	0.44
24:1Y:132:TRP:CE3	82:1Y:203:PGT:H121	2.53	0.44
82:1Y:203:PGT:H131	82:1Y:203:PGT:H32	1.99	0.44
30:1e:57:ILE:HG13	30:1e:58:GLU:N	2.29	0.44
33:1h:114:MET:SD	33:1h:120:GLY:HA3	2.57	0.44
40:1o:44:GLU:H	40:1o:44:GLU:HG3	1.61	0.44
75:1q:202:CDL:H531	75:1q:202:CDL:CB7	2.48	0.44
45:3A:244:ARG:HD3	51:3G:12:MET:HE2	1.98	0.44
45:3A:368:HIS:C	45:3A:370:ASP:N	2.76	0.44
45:3A:446:PHE:HA	54:3Y:20:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:37:LEU:HD13	85:3C:502:HEM:C3B	2.53	0.44
47:3C:119:LEU:O	47:3C:123:VAL:HG23	2.18	0.44
47:3C:156:ILE:O	47:3C:160:LEU:HB2	2.17	0.44
47:3C:245:PHE:CE1	48:3D:105:LEU:HG	2.53	0.44
45:3N:2:ALA:HB2	46:3O:41:TYR:CE1	2.53	0.44
45:3N:211:LEU:HA	45:3N:214:LYS:HG2	2.00	0.44
69:3P:508:3PE:H2H2	69:3P:519:3PE:H3I3	1.98	0.44
48:3Q:153:PHE:O	48:3Q:156:GLN:N	2.42	0.44
49:3R:211:VAL:C	49:3R:212:ILE:HD12	2.43	0.44
49:3R:266:THR:OG1	49:3R:270:LEU:HB2	2.17	0.44
69:3T:103:3PE:H3A1	69:3T:103:3PE:H3D2	1.54	0.44
54:3X:3:SER:HA	54:3X:6:LEU:CB	2.46	0.44
54:3Y:13:LEU:HB3	75:3Y:106:CDL:C14	2.48	0.44
55:4A:446:ALA:HB1	56:4B:2:ALA:O	2.18	0.44
55:4A:468:MET:HE2	55:4A:472:ILE:HG13	1.98	0.44
93:4B:303:PSC:H061	59:4E:40:ASP:CB	2.48	0.44
57:4C:58:TRP:NE1	91:4C:305:PGV:H221	2.33	0.44
70:1B:203:PC1:H352	70:1B:203:PC1:H381	1.85	0.44
5:1E:68:LYS:HE3	5:1E:68:LYS:HB2	1.83	0.44
6:1F:384:ALA:HB1	6:1F:388:GLU:HG3	2.00	0.44
7:1G:98:LEU:HD12	7:1G:98:LEU:HA	1.87	0.44
7:1G:283:MET:HB2	7:1G:560:ILE:HB	2.00	0.44
8:1H:277:TYR:CD2	70:1H:402:PC1:H272	2.53	0.44
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.52	0.44
12:1L:65:ASN:ND2	75:1i:201:CDL:H391	2.33	0.44
12:1L:244:SER:O	12:1L:249:SER:HB3	2.18	0.44
13:1M:98:MET:HE2	13:1M:98:MET:HA	1.99	0.44
14:1N:278:MET:HE3	14:1N:278:MET:HB3	1.72	0.44
18:1R:27:ARG:HE	18:1R:27:ARG:HB3	1.62	0.44
21:1V:75:GLN:O	21:1V:78:GLU:HG2	2.18	0.44
69:1Y:214:3PE:C3H	75:3P:513:CDL:H171	2.43	0.44
69:1Y:216:3PE:H362	69:1Y:216:3PE:H331	1.82	0.44
31:1f:14:ILE:HD13	69:1f:101:3PE:H2D1	1.99	0.44
69:1m:201:3PE:H241	69:1m:201:3PE:H272	1.75	0.44
75:3A:501:CDL:OB7	75:3A:501:CDL:H152	2.18	0.44
46:3B:312:PHE:HD2	49:3I:60:ALA:O	2.01	0.44
49:3E:177:ARG:HG2	49:3E:178:HIS:N	2.30	0.44
69:3G:109:3PE:H331	69:3G:109:3PE:H361	1.68	0.44
45:3N:146:ARG:O	45:3N:149:VAL:HG12	2.18	0.44
46:3O:78:LYS:CG	46:3O:129:ALA:HB1	2.48	0.44
46:3O:314:ALA:HA	49:3V:63:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3P:517:3PE:H392	69:3P:518:3PE:C2E	2.48	0.44
49:3R:122:THR:HB	53:3W:25:ILE:HG12	2.00	0.44
49:3R:212:ILE:CG2	49:3R:263:TYR:HD2	2.31	0.44
54:3X:20:THR:HG22	54:3X:24:TRP:CD1	2.53	0.44
75:3Y:106:CDL:H131	75:3Y:106:CDL:H322	1.99	0.44
75:4B:302:CDL:H652	75:4B:302:CDL:H421	2.00	0.44
91:4C:303:PGV:H342	91:4C:303:PGV:H172	2.00	0.44
62:4H:56:TYR:CE2	68:4N:80:PRO:HD2	2.52	0.44
62:4H:57:ARG:O	62:4H:61:LYS:HB2	2.18	0.44
2:1B:96:MET:O	2:1B:96:MET:HG3	2.17	0.44
2:1B:166:LYS:HE2	2:1B:166:LYS:HB3	1.71	0.44
3:1C:92:ILE:HD11	3:1C:140:VAL:HG11	2.00	0.44
4:1D:18:VAL:CG2	14:1N:171:ASN:CG	2.91	0.44
4:1D:83:LEU:O	4:1D:83:LEU:HG	2.17	0.44
4:1D:427:GLU:O	4:1D:430:ARG:NH1	2.50	0.44
7:1G:215:PHE:HD1	9:1I:104:ARG:HH11	1.64	0.44
7:1G:251:LEU:HD21	17:1Q:45:MET:HE2	1.99	0.44
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.83	0.44
69:1L:706:3PE:H3B2	69:1L:706:3PE:H381	1.79	0.44
14:1N:84:TRP:HB2	30:1e:18:THR:HA	1.99	0.44
15:1O:34:GLY:O	15:1O:35:LYS:C	2.58	0.44
16:1P:179:LEU:H	16:1P:179:LEU:HD23	1.83	0.44
16:1P:271:GLU:OE2	16:1P:281:ARG:HD3	2.18	0.44
17:1Q:125:ASN:O	44:1s:70:ARG:NE	2.50	0.44
20:1T:24:LYS:HA	20:1T:24:LYS:HD3	1.63	0.44
24:1Y:27:ILE:CD1	69:1Y:208:3PE:H3I2	2.48	0.44
24:1Y:79:VAL:CG1	69:1Y:214:3PE:O31	2.58	0.44
24:1Y:111:ALA:O	70:1Y:206:PC1:H292	2.18	0.44
69:1Y:214:3PE:C3I	75:3P:513:CDL:H712	2.48	0.44
69:1Z:201:3PE:H2B2	69:1Z:201:3PE:H281	1.85	0.44
69:1f:101:3PE:H3D2	69:1f:101:3PE:H3A1	1.71	0.44
38:1m:3:PRO:HD2	39:1n:72:TYR:CE1	2.53	0.44
38:1m:6:LYS:H	38:1m:6:LYS:HG2	1.69	0.44
45:3A:48:GLU:OE2	45:3A:53:ASN:HA	2.18	0.44
69:3A:502:3PE:H3D1	69:3E:303:3PE:H3B1	1.99	0.44
47:3C:171:ASP:OD1	47:3C:172:LYS:N	2.50	0.44
47:3C:359:PHE:CE1	69:3C:511:3PE:H3E1	2.52	0.44
69:3C:509:3PE:C3F	75:3N:502:CDL:H871	2.47	0.44
69:3C:515:3PE:H11	69:3C:516:3PE:H12	2.00	0.44
49:3E:169:TRP:CB	49:3E:174:LEU:HD22	2.47	0.44
49:3E:200:HIS:CG	49:3E:201:ASP:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3E:302:3PE:H222	69:3E:302:3PE:H252	1.78	0.44
48:3Q:131:LEU:HB3	48:3Q:164:ILE:HD11	1.99	0.44
49:3R:164:ASN:O	49:3R:165:MET:C	2.61	0.44
51:3T:70:LYS:HB3	51:3T:70:LYS:HE2	1.74	0.44
55:4A:374:VAL:HA	55:4A:377:PHE:CE2	2.53	0.44
57:4C:206:LEU:HD23	57:4C:206:LEU:HA	1.89	0.44
58:4D:122:ARG:HG3	65:4K:53:TRP:CD2	2.53	0.44
60:4F:93:SER:O	60:4F:94:HIS:HB3	2.18	0.44
69:4G:101:3PE:H341	69:4G:104:3PE:H241	2.00	0.44
68:4N:33:VAL:HG21	91:4N:101:PGV:H72	2.00	0.44
1:1A:84:LEU:HD23	1:1A:84:LEU:HA	1.89	0.43
6:1F:296:ALA:HB1	6:1F:306:LEU:HD12	2.00	0.43
6:1F:350:LEU:HD12	6:1F:350:LEU:HA	1.87	0.43
7:1G:331:LEU:HD22	7:1G:525:LEU:HD22	2.00	0.43
7:1G:478:ARG:HH11	7:1G:478:ARG:HG3	1.83	0.43
10:1J:99:MET:CE	69:1J:201:3PE:C3E	2.94	0.43
12:1L:78:LEU:HD11	75:1L:704:CDL:H873	1.99	0.43
12:1L:534:HIS:CG	69:1L:701:3PE:H31	2.53	0.43
69:1L:712:3PE:C3	69:1L:204:3PE:H332	2.48	0.43
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	2.00	0.43
19:1S:31:GLY:HA3	19:1S:81:PHE:O	2.17	0.43
20:1T:70:LEU:HD21	20:1T:79:TYR:CD2	2.53	0.43
23:1X:162:HIS:CE1	33:1h:96:ILE:HB	2.53	0.43
69:1Y:215:3PE:C3D	47:3P:357:LEU:CD2	2.96	0.43
75:1Y:217:CDL:H611	75:1Y:217:CDL:H431	2.00	0.43
27:1b:26:GLY:CA	69:1b:101:3PE:H2C2	2.39	0.43
31:1f:17:PRO:HB2	69:1f:102:3PE:H2G2	2.00	0.43
75:1g:201:CDL:H132	33:1h:28:TYR:OH	2.17	0.43
69:1k:101:3PE:H391	69:1k:101:3PE:H362	1.76	0.43
39:1n:100:GLU:H	39:1n:100:GLU:HG3	1.62	0.43
39:1n:163:PRO:HA	39:1n:164:PRO:HD3	1.93	0.43
40:1o:80:LYS:HB2	40:1o:80:LYS:HE2	1.67	0.43
47:3C:176:THR:HG23	47:3P:53:MET:O	2.17	0.43
69:3C:503:3PE:H2B2	69:3C:503:3PE:H281	1.83	0.43
69:3C:509:3PE:H3E1	54:3X:29:ALA:HA	1.99	0.43
49:3E:212:ILE:HB	49:3E:263:TYR:CE2	2.53	0.43
50:3F:105:TYR:O	50:3F:109:VAL:HG23	2.17	0.43
69:3G:101:3PE:H371	69:3G:101:3PE:H2B2	2.00	0.43
46:3O:120:MET:HE3	46:3O:219:VAL:HG11	1.99	0.43
69:3P:507:3PE:H221	69:3P:507:3PE:H252	1.73	0.43
48:3Q:134:TYR:CG	48:3Q:162:PRO:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3Q:229:VAL:CG2	51:3T:20:PRO:HD3	2.48	0.43
69:3Q:502:3PE:H282	69:3Q:503:3PE:H292	1.99	0.43
69:3Q:504:3PE:H331	69:3Q:504:3PE:H11	2.00	0.43
49:3R:234:TYR:CD2	49:3R:243:TYR:HB2	2.53	0.43
49:3R:235:TYR:CB	49:3R:242:HIS:HB3	2.41	0.43
50:3S:77:LYS:HA	50:3S:80:TRP:CD2	2.52	0.43
55:4A:219:PHE:HE1	57:4C:196:THR:HG22	1.82	0.43
55:4A:423:MET:SD	91:4K:101:PGV:H341	2.58	0.43
56:4B:161:HIS:CE1	56:4B:200:CYS:HB2	2.52	0.43
57:4C:90:GLU:O	57:4C:93:PHE:HB3	2.18	0.43
57:4C:140:SER:HB2	57:4C:242:TRP:HE1	1.83	0.43
91:4C:303:PGV:H282	68:4N:45:TRP:HH2	1.83	0.43
58:4D:77:GLU:HG3	65:4K:10:HIS:CE1	2.53	0.43
68:4N:33:VAL:HG23	91:4N:101:PGV:H41	2.00	0.43
70:1B:203:PC1:C2A	8:1H:46:LEU:HD21	2.44	0.43
69:1B:205:3PE:H31	75:1q:202:CDL:H521	0.70	0.43
4:1D:157:HIS:O	4:1D:161:ILE:HG12	2.18	0.43
7:1G:144:PRO:HD2	7:1G:192:MET:HE1	2.00	0.43
7:1G:366:THR:O	7:1G:367:THR:OG1	2.33	0.43
10:1J:34:ILE:HG13	10:1J:35:VAL:N	2.33	0.43
10:1J:95:SER:HB2	69:1J:201:3PE:C3E	2.45	0.43
69:1N:401:3PE:H352	69:1N:401:3PE:H382	1.71	0.43
15:1O:50:HIS:NE2	15:1O:125:GLU:OE1	2.52	0.43
70:1Y:207:PC1:P	70:1Y:207:PC1:H152	2.58	0.43
28:1c:39:VAL:HG23	28:1c:40:LEU:HD22	1.99	0.43
32:1g:63:PHE:CE2	75:1g:201:CDL:H221	2.41	0.43
75:1g:201:CDL:H602	75:1g:201:CDL:H571	1.52	0.43
69:1l:203:3PE:H221	69:1l:203:3PE:H251	1.62	0.43
42:1q:55:PHE:CD1	43:1r:25:LEU:HB3	2.53	0.43
44:1s:71:GLN:HB2	44:1s:75:HIS:CD2	2.52	0.43
45:3A:82:MET:HE3	45:3A:84:ALA:CB	2.48	0.43
45:3A:349:ALA:HB3	45:3A:408:ARG:HG3	1.99	0.43
69:3A:502:3PE:H2A2	69:3A:502:3PE:H272	1.72	0.43
69:3A:502:3PE:C3D	69:3E:303:3PE:H3B1	2.47	0.43
47:3C:29:SER:O	47:3C:32:ASN:HB2	2.18	0.43
47:3C:272:TRP:HA	47:3C:275:LEU:HG	2.00	0.43
47:3C:333:ILE:HG23	69:3C:503:3PE:H341	1.99	0.43
48:3D:171:ARG:HH12	48:3D:174:LYS:HG3	1.81	0.43
49:3E:222:CYS:C	49:3E:238:CYS:HB3	2.43	0.43
49:3E:224:PRO:HB3	49:3E:236:CYS:SG	2.57	0.43
49:3E:263:TYR:HB2	49:3E:272:ILE:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:136:GLN:HA	45:3N:139:GLN:OE1	2.18	0.43
46:3O:111:CYS:HB2	46:3O:119:LEU:HD22	2.00	0.43
47:3P:46:LEU:HD21	69:3R:302:3PE:H2D2	2.00	0.43
47:3P:95:PHE:CE1	69:3P:519:3PE:H3F1	2.53	0.43
48:3Q:63:ALA:O	48:3Q:67:GLU:HG3	2.18	0.43
69:3Q:503:3PE:H341	69:3Q:503:3PE:H271	2.01	0.43
49:3R:167:PHE:HE2	49:3R:176:VAL:HB	1.83	0.43
49:3R:213:LEU:O	49:3R:214:ILE:C	2.60	0.43
49:3R:229:GLY:HA2	49:3R:234:TYR:C	2.44	0.43
69:3X:107:3PE:O21	69:3X:107:3PE:C24	2.66	0.43
55:4A:65:MET:HB3	88:4A:601:HEA:HBC1	2.00	0.43
91:4J:101:PGV:H242	91:4J:101:PGV:H211	1.90	0.43
70:1A:202:PC1:O13	70:1A:202:PC1:H133	2.19	0.43
69:1A:203:3PE:H2B2	69:1A:203:3PE:H3A1	2.00	0.43
6:1F:47:GLU:O	6:1F:51:LYS:HG2	2.18	0.43
8:1H:82:ALA:HB1	8:1H:229:ALA:HB3	2.00	0.43
8:1H:173:TRP:HE1	70:1H:404:PC1:C12	2.31	0.43
75:1H:401:CDL:OA9	75:1H:401:CDL:OA5	2.36	0.43
10:1J:167:VAL:HG22	14:1N:42:PRO:HG2	1.99	0.43
12:1L:7:LEU:HD22	12:1L:46:LEU:HD21	2.00	0.43
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.32	0.43
13:1M:95:TYR:CE1	13:1M:132:ILE:HD12	2.54	0.43
70:1M:501:PC1:H2D2	70:1M:501:PC1:H2G1	1.58	0.43
14:1N:203:LEU:HD13	70:1d:204:PC1:H3D1	2.00	0.43
16:1P:203:GLN:OE1	16:1P:235:ARG:NH1	2.50	0.43
20:1T:22:TYR:HE1	20:1T:24:LYS:HB2	1.82	0.43
20:1U:19:LEU:HB2	20:1U:30:LEU:HD21	2.00	0.43
24:1Y:62:SER:HB3	69:1Y:208:3PE:H372	1.82	0.43
69:1Z:201:3PE:H112	69:1Z:201:3PE:C1	2.45	0.43
29:1d:33:TYR:CD1	75:1d:202:CDL:C41	2.99	0.43
75:1g:201:CDL:H262	75:1g:201:CDL:H461	2.01	0.43
75:1i:201:CDL:C56	41:1p:44:VAL:HG12	2.44	0.43
37:1l:139:TYR:CG	37:1l:150:PRO:HG3	2.54	0.43
45:3A:398:ARG:HA	45:3A:401:GLU:OE2	2.18	0.43
47:3C:114:ASN:ND2	69:3C:514:3PE:H32	2.33	0.43
47:3C:323:CYS:SG	69:3G:109:3PE:H31	2.58	0.43
46:3O:120:MET:CE	46:3O:219:VAL:HG11	2.47	0.43
46:3O:327:ILE:HD12	49:3V:58:GLN:HB3	2.00	0.43
47:3P:278:TYR:O	47:3P:282:ARG:HG3	2.17	0.43
47:3P:286:ASN:ND2	69:3P:503:3PE:O14	2.46	0.43
48:3Q:12:TRP:HD1	48:3Q:15:ARG:HH21	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3Q:118:ARG:HG3	48:3Q:194:SER:CB	2.38	0.43
69:3Q:503:3PE:H332	69:3Q:503:3PE:C23	2.48	0.43
49:3R:268:ASP:O	49:3R:271:VAL:HG22	2.17	0.43
69:3R:304:3PE:H332	69:3R:304:3PE:H362	1.77	0.43
54:3Y:44:TRP:HB3	69:3Y:105:3PE:H3A2	2.00	0.43
91:4J:101:PGV:H81	91:4J:101:PGV:H272	2.00	0.43
1:1A:3:ILE:O	1:1A:6:THR:HG23	2.17	0.43
6:1F:423:ARG:N	6:1F:424:PRO:HD2	2.34	0.43
8:1H:52:ALA:O	8:1H:56:VAL:HG13	2.18	0.43
8:1H:63:PRO:HB2	8:1H:66:SER:HB3	2.00	0.43
9:1I:80:CYS:O	9:1I:81:LYS:HB2	2.18	0.43
9:1I:169:ILE:O	9:1I:173:TYR:N	2.48	0.43
10:1J:66:VAL:O	10:1J:70:TYR:N	2.48	0.43
12:1L:188:TRP:CD1	12:1L:211:MET:HE3	2.53	0.43
69:1L:711:3PE:H2C1	69:1L:712:3PE:H3C2	2.01	0.43
13:1M:53:SER:C	13:1M:55:THR:H	2.24	0.43
24:1Y:37:ALA:HB2	69:1Y:210:3PE:H3C1	2.00	0.43
75:1Y:217:CDL:H201	75:1Y:217:CDL:H172	1.54	0.43
69:1d:203:3PE:H3A1	69:1d:203:3PE:H3D2	1.70	0.43
34:1i:92:LYS:HE2	34:1i:95:THR:HG21	2.00	0.43
37:1l:54:SER:HB2	37:1l:91:THR:H	1.84	0.43
37:1l:121:ILE:HG13	37:1l:122:TYR:CD1	2.53	0.43
43:1r:63:MET:HE3	43:1r:63:MET:HB3	1.85	0.43
75:3A:501:CDL:H272	75:3A:501:CDL:H212	2.00	0.43
69:3A:503:3PE:H2	69:3A:503:3PE:H222	1.79	0.43
46:3B:40:ASN:O	46:3B:41:TYR:HB2	2.17	0.43
46:3B:95:LYS:HZ3	46:3B:96:LEU:C	2.27	0.43
46:3B:154:ASN:ND2	49:3I:78:TYR:CE1	2.86	0.43
48:3D:309:TYR:CE2	51:3G:28:PHE:HE2	2.36	0.43
69:3D:503:3PE:H271	69:3G:102:3PE:C38	2.49	0.43
49:3E:254:ALA:O	49:3E:255:PRO:C	2.58	0.43
53:3J:53:TRP:O	53:3J:54:LYS:HB3	2.18	0.43
45:3N:350:THR:O	45:3N:353:GLU:HG2	2.18	0.43
46:3O:116:ILE:HG23	46:3O:120:MET:HG3	1.99	0.43
46:3O:219:VAL:HA	46:3O:222:ARG:CG	2.49	0.43
47:3P:11:MET:HA	47:3P:14:ILE:HG23	1.99	0.43
47:3P:324:LEU:HD23	47:3P:327:MET:SD	2.58	0.43
69:3P:503:3PE:H282	69:3P:518:3PE:C34	2.48	0.43
69:3P:510:3PE:H2I3	51:3T:54:VAL:HG22	1.99	0.43
75:3P:513:CDL:H472	69:3P:520:3PE:H332	2.00	0.43
48:3Q:210:MET:HE3	53:3W:36:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
70:3R:303:PC1:H142	70:3R:303:PC1:H112	1.58	0.43
51:3T:32:LYS:C	51:3T:35:PRO:HD2	2.44	0.43
53:3W:9:ARG:N	53:3W:9:ARG:CD	2.80	0.43
91:4A:609:PGV:O04	66:4L:24:MET:HB2	2.19	0.43
91:4A:609:PGV:H281	66:4L:28:TYR:HD2	1.82	0.43
75:4C:306:CDL:H562	75:4C:306:CDL:H741	1.99	0.43
4:1D:8:VAL:O	4:1D:12:GLU:HG2	2.19	0.43
6:1F:46:LYS:NZ	6:1F:167:CYS:O	2.34	0.43
6:1F:343:ILE:HD12	6:1F:344:VAL:HG23	2.00	0.43
7:1G:199:ILE:HA	7:1G:202:ILE:HG12	2.00	0.43
7:1G:258:ILE:HD11	7:1G:579:ARG:HD3	2.00	0.43
8:1H:261:LEU:HD12	70:1H:404:PC1:H321	2.00	0.43
12:1L:27:TYR:O	12:1L:115:ASN:ND2	2.46	0.43
12:1L:78:LEU:HD11	75:1L:704:CDL:C86	2.48	0.43
69:1L:705:3PE:H3F2	82:1Y:203:PGT:H452	2.00	0.43
13:1M:123:GLU:HA	13:1M:126:LEU:HD13	2.00	0.43
14:1N:8:THR:HG22	75:1N:402:CDL:C40	2.47	0.43
14:1N:239:VAL:HG11	29:1d:47:ALA:HB1	2.00	0.43
16:1P:99:TRP:CZ2	16:1P:276:GLU:HA	2.53	0.43
20:1T:37:MET:HE2	20:1T:71:MET:HE1	1.99	0.43
22:1W:91:GLU:OE1	22:1W:94:ILE:HD11	2.19	0.43
24:1Y:108:GLY:CA	70:1Y:206:PC1:H31	2.48	0.43
75:1Y:217:CDL:H542	75:1Y:217:CDL:H571	1.68	0.43
27:1b:23:ALA:HA	69:1b:101:3PE:H2A1	1.99	0.43
32:1g:63:PHE:HB2	75:1g:201:CDL:H141	2.01	0.43
33:1h:50:ALA:HB2	41:1p:60:TYR:HE1	1.83	0.43
37:1l:10:PRO:HB2	38:1m:74:ASN:HD22	1.84	0.43
37:1l:12:PRO:O	37:1l:46:ASP:HB3	2.19	0.43
48:3D:166:GLY:HA2	48:3Q:99:GLU:HB2	1.99	0.43
52:3H:64:LEU:HD12	52:3H:64:LEU:HA	1.76	0.43
52:3H:72:ARG:HD2	52:3H:77:GLU:OE1	2.19	0.43
53:3J:58:HIS:CA	53:3J:60:TYR:N	2.81	0.43
46:3O:39:GLU:CD	46:3O:113:ARG:HH22	2.26	0.43
47:3P:285:PRO:HG3	69:3P:517:3PE:O14	2.18	0.43
47:3P:327:MET:HE1	70:3T:102:PC1:H3D1	2.00	0.43
75:3P:513:CDL:H612	75:3T:101:CDL:C34	2.47	0.43
49:3R:128:ALA:CB	69:3R:302:3PE:H361	2.37	0.43
49:3R:191:GLU:CD	49:3R:192:VAL:H	2.27	0.43
49:3R:223:VAL:HG23	49:3R:223:VAL:O	2.18	0.43
69:3R:304:3PE:H32	70:3X:104:PC1:H251	1.99	0.43
55:4A:289:ALA:O	55:4A:290:HIS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
93:4B:303:PSC:H083	63:4I:14:ALA:HB2	2.00	0.43
58:4D:121:LYS:HG3	65:4K:53:TRP:CD1	2.54	0.43
6:1F:279:LEU:HD12	6:1F:279:LEU:HA	1.87	0.43
7:1G:148:THR:HG22	7:1G:208:LEU:CD2	2.49	0.43
7:1G:534:ARG:HH22	42:1q:145:LYS:HE3	1.84	0.43
9:1I:74:GLU:HG3	9:1I:75:GLU:N	2.32	0.43
10:1J:156:VAL:O	10:1J:160:SER:OG	2.34	0.43
12:1L:512:LYS:HG2	64:4J:16:ASN:ND2	2.27	0.43
12:1L:517:SER:HB3	69:1L:708:3PE:O22	2.19	0.43
12:1L:528:TYR:CD1	37:1l:101:MET:HG2	2.54	0.43
13:1M:143:LEU:HD11	14:1N:303:THR:HG21	2.01	0.43
14:1N:277:ILE:HG12	82:1Y:203:PGT:H161	1.98	0.43
75:1N:402:CDL:H552	69:1e:201:3PE:O32	2.18	0.43
15:1O:174:VAL:HG22	15:1O:225:ALA:HB2	2.01	0.43
15:1O:211:LEU:O	15:1O:215:SER:OG	2.36	0.43
16:1P:57:MET:O	16:1P:60:ARG:HG3	2.19	0.43
16:1P:200:THR:HA	16:1P:290:SER:OG	2.18	0.43
70:1Y:207:PC1:H3B2	70:1Y:207:PC1:H3F2	2.00	0.43
70:1Y:207:PC1:C31	70:3T:102:PC1:H153	2.48	0.43
69:1Y:208:3PE:H221	69:1Y:208:3PE:H251	1.81	0.43
29:1d:34:MET:HE1	69:1d:203:3PE:H2F1	1.99	0.43
69:1g:202:3PE:H331	69:1g:202:3PE:H232	2.01	0.43
33:1h:36:VAL:HG13	70:1h:203:PC1:H3G1	2.01	0.43
70:1h:202:PC1:H222	69:1h:204:3PE:H332	2.00	0.43
38:1m:99:PHE:CD2	69:1m:205:3PE:C3I	3.01	0.43
38:1m:106:THR:HG23	38:1m:110:LYS:HE3	2.00	0.43
45:3A:445:ARG:HH12	75:3A:501:CDL:HB21	1.84	0.43
46:3B:232:LEU:HA	46:3B:232:LEU:HD23	1.80	0.43
47:3C:33:PHE:O	47:3C:37:LEU:HG	2.19	0.43
69:3C:510:3PE:H32	51:3G:46:CYS:SG	2.58	0.43
48:3D:226:PRO:O	48:3D:229:VAL:HG13	2.18	0.43
49:3E:169:TRP:CD2	49:3E:273:VAL:HA	2.53	0.43
46:3O:29:LEU:HB3	46:3O:30:PRO:HD2	2.01	0.43
47:3P:296:ALA:O	47:3P:300:ILE:HB	2.18	0.43
69:3P:507:3PE:H231	69:3P:507:3PE:H371	2.01	0.43
69:3P:511:3PE:H222	69:3X:105:3PE:H322	2.00	0.43
69:3P:514:3PE:H321	69:3P:514:3PE:H352	1.87	0.43
53:3W:20:THR:OG1	54:3X:23:MET:HE2	2.18	0.43
69:3Y:101:3PE:C2H	69:3Y:104:3PE:H3B2	2.42	0.43
69:3Y:107:3PE:H361	69:3Y:107:3PE:H391	1.70	0.43
91:4C:301:PGV:H171	91:4G:102:PGV:C34	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:4C:304:PGV:H343	75:4C:307:CDL:H471	2.00	0.43
63:4I:27:VAL:O	63:4I:31:VAL:HG23	2.18	0.43
3:1C:40:VAL:HG12	3:1C:50:ILE:HG23	2.00	0.43
7:1G:518:PRO:HB2	7:1G:538:PRO:HD3	2.00	0.43
8:1H:269:THR:HG21	70:1H:404:PC1:H3F2	2.00	0.43
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.18	0.43
12:1L:346:ILE:HA	12:1L:366:MET:HE1	1.99	0.43
69:1L:712:3PE:H2E2	69:1L:712:3PE:H2H1	1.67	0.43
13:1M:1:FME:CE	13:1M:111:THR:HG21	2.48	0.43
16:1P:99:TRP:CD1	16:1P:277:PRO:HD2	2.54	0.43
69:1Y:201:3PE:H3A1	69:1Y:201:3PE:C26	2.35	0.43
29:1d:33:TYR:CE1	75:1d:202:CDL:H411	2.53	0.43
40:1o:103:ARG:HE	40:1o:107:LEU:HD12	1.83	0.43
43:1r:2:SER:CB	43:1r:27:TYR:HE2	2.32	0.43
45:3A:199:ALA:HB3	45:3A:208:LEU:HD22	2.00	0.43
45:3A:358:LYS:HE3	45:3A:399:ILE:O	2.19	0.43
46:3B:83:PHE:CE2	50:3S:104:ARG:HG3	2.54	0.43
46:3B:279:LEU:HB3	46:3B:295:LEU:HG	2.00	0.43
47:3C:353:LEU:HD11	69:3G:111:3PE:H291	2.01	0.43
48:3D:299:MET:HE1	69:3J:104:3PE:H3B1	2.00	0.43
75:3F:201:CDL:H721	75:3F:201:CDL:H752	1.65	0.43
51:3G:20:LEU:HG	51:3G:24:GLU:HB2	2.00	0.43
53:3J:43:ILE:CG1	69:3J:104:3PE:H331	2.49	0.43
45:3N:191:LYS:HB3	45:3N:191:LYS:HE3	1.84	0.43
47:3P:302:ILE:O	47:3P:306:MET:HE3	2.19	0.43
69:3P:503:3PE:H231	69:3P:518:3PE:O32	2.18	0.43
48:3Q:21:LEU:HB2	48:3Q:26:ILE:HD11	2.01	0.43
49:3R:222:CYS:HB3	49:3R:238:CYS:HB3	1.45	0.43
49:3R:248:ARG:HD3	49:3R:257:ASN:HD22	1.84	0.43
50:3S:45:GLU:OE2	50:3S:48:ARG:NH1	2.52	0.43
54:3X:39:ARG:O	54:3X:40:LEU:C	2.60	0.43
69:3X:105:3PE:H262	69:3X:105:3PE:H391	2.01	0.43
55:4A:351:GLY:HA3	55:4A:380:VAL:HG13	2.01	0.43
91:4A:606:PGV:H101	58:4D:84:THR:HG22	2.01	0.43
75:4B:302:CDL:H222	75:4B:302:CDL:OA7	2.17	0.43
68:4N:32:TYR:C	68:4N:34:THR:H	2.27	0.43
70:1B:203:PC1:H153	70:1B:203:PC1:H112	1.46	0.43
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.48	0.43
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	2.00	0.43
70:1J:202:PC1:H322	70:1J:202:PC1:H351	1.78	0.43
12:1L:488:MET:HE3	12:1L:488:MET:HB3	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:571:MET:O	12:1L:575:ILE:HG13	2.18	0.43
75:1L:704:CDL:H841	75:1L:704:CDL:H872	1.64	0.43
69:1L:709:3PE:H271	69:1L:709:3PE:H242	1.78	0.43
69:1M:502:3PE:H351	69:1M:502:3PE:H382	1.69	0.43
17:1Q:34:LYS:HE2	17:1Q:34:LYS:HB2	1.80	0.43
75:1d:205:CDL:H771	75:1d:205:CDL:C23	2.49	0.43
32:1g:101:GLU:HG3	32:1g:107:LEU:HD23	1.99	0.43
47:3C:11:MET:CE	69:3C:516:3PE:H352	2.48	0.43
47:3C:131:TYR:O	47:3C:139:SER:OG	2.33	0.43
48:3D:229:VAL:HG11	52:3H:80:THR:HG22	2.00	0.43
49:3E:184:ILE:O	49:3E:185:ASP:C	2.59	0.43
49:3E:209:GLU:O	49:3E:210:TRP:CG	2.71	0.43
49:3E:214:ILE:HG22	49:3E:216:VAL:HG23	2.00	0.43
49:3E:235:TYR:CD1	49:3E:236:CYS:N	2.87	0.43
49:3E:235:TYR:HD1	49:3E:242:HIS:HA	1.83	0.43
45:3N:42:ASP:HB2	45:3N:194:ARG:HB3	1.99	0.43
46:3O:35:ILE:HD11	46:3O:220:ALA:HB2	2.00	0.43
47:3P:14:ILE:HD12	47:3P:14:ILE:O	2.19	0.43
47:3P:155:TYR:HE2	69:3P:507:3PE:C21	2.32	0.43
47:3P:207:ASN:ND2	47:3P:211:ILE:O	2.52	0.43
70:3P:509:PC1:H3F2	70:3P:509:PC1:H3I3	1.80	0.43
75:3P:513:CDL:H472	69:3P:520:3PE:C34	2.49	0.43
69:3P:515:3PE:H2H1	69:3P:516:3PE:H3D2	1.99	0.43
48:3Q:127:VAL:O	48:3Q:131:LEU:HG	2.19	0.43
49:3R:152:ILE:C	49:3R:153:GLU:HG2	2.44	0.43
69:3R:305:3PE:H32	51:3T:26:PHE:CD1	2.49	0.43
69:3W:101:3PE:H3E2	69:3W:102:3PE:H261	1.99	0.43
69:3W:102:3PE:C3	69:3W:102:3PE:H342	2.49	0.43
56:4B:103:GLN:HA	56:4B:104:TRP:HA	1.82	0.43
75:4C:307:CDL:H242	75:4C:307:CDL:H652	2.01	0.43
7:1G:156:CYS:SG	7:1G:157:THR:N	2.92	0.43
8:1H:47:GLN:N	8:1H:48:PRO:CD	2.81	0.43
8:1H:187:ILE:HG12	70:1H:402:PC1:H251	2.00	0.43
70:1H:403:PC1:H132	25:1Z:144:THR:CG2	2.48	0.43
10:1J:169:MET:O	10:1J:173:ARG:N	2.32	0.43
12:1L:24:SER:CA	69:1L:710:3PE:O14	2.67	0.43
12:1L:103:PHE:HB2	12:1L:341:MET:HE3	2.00	0.43
12:1L:411:MET:HE2	12:1L:411:MET:HA	2.01	0.43
13:1M:7:PRO:HG3	31:1f:20:PHE:CA	2.49	0.43
13:1M:227:GLY:O	13:1M:231:LEU:HD12	2.17	0.43
15:1O:54:ALA:HB3	15:1O:104:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:84:ASP:HB3	24:1Y:129:LEU:HD11	2.00	0.43
69:1Y:208:3PE:H3C1	69:1Y:208:3PE:H391	1.86	0.43
69:1Y:211:3PE:H221	69:1Y:211:3PE:H2	1.85	0.43
69:1Y:215:3PE:H281	69:1Y:215:3PE:H251	1.56	0.43
25:1Z:131:GLU:CD	25:1Z:131:GLU:H	2.26	0.43
75:1d:202:CDL:H631	75:1d:202:CDL:H421	2.00	0.43
42:1q:20:LEU:O	42:1q:24:LEU:HG	2.19	0.43
52:3H:50:GLU:HG2	52:3H:86:PHE:HZ	1.84	0.43
49:3I:41:PRO:HB2	49:3I:44:ASP:HB2	2.00	0.43
69:3J:101:3PE:H2C1	69:3J:101:3PE:H2F2	1.66	0.43
45:3N:316:GLU:OE1	45:3N:316:GLU:N	2.52	0.43
45:3N:390:ILE:HG23	45:3N:394:GLU:CD	2.44	0.43
46:3O:329:GLN:O	46:3O:330:ALA:C	2.61	0.43
47:3P:50:PHE:CG	49:3R:136:PHE:HD2	2.37	0.43
47:3P:137:GLN:O	47:3P:141:TRP:HD1	2.02	0.43
47:3P:265:PRO:CD	47:3P:268:ILE:HD11	2.48	0.43
47:3P:281:LEU:C	47:3P:281:LEU:HD13	2.44	0.43
47:3P:303:LEU:HD22	47:3P:303:LEU:N	2.34	0.43
69:3P:506:3PE:H2F2	69:3P:506:3PE:H2C1	1.83	0.43
48:3Q:93:LYS:HG3	48:3Q:94:PRO:HD2	2.01	0.43
49:3R:212:ILE:HB	49:3R:265:PHE:CE1	2.54	0.43
69:3R:302:3PE:H2A1	69:3R:302:3PE:H272	1.71	0.43
69:3R:305:3PE:H251	69:3R:305:3PE:H281	1.92	0.43
50:3S:82:LYS:HB3	50:3S:84:GLU:OE1	2.19	0.43
52:3U:45:SER:C	52:3U:47:ARG:H	2.27	0.43
55:4A:1:FME:HCN	91:4A:609:PGV:C05	2.44	0.43
55:4A:25:TRP:CG	91:4A:609:PGV:H312	2.54	0.43
56:4B:161:HIS:HB2	56:4B:174:ALA:HB3	2.01	0.43
62:4H:46:LYS:HG3	62:4H:47:GLY:N	2.33	0.43
68:4N:36:LEU:O	68:4N:40:ASN:HB2	2.19	0.43
1:1A:95:LEU:HA	1:1A:98:LEU:HB2	2.01	0.43
2:1B:84:ASP:OD1	8:1H:58:LYS:NZ	2.48	0.43
3:1C:131:GLU:HG2	3:1C:142:PHE:CE1	2.54	0.43
4:1D:35:ASP:CG	14:1N:176:ARG:HH22	2.27	0.43
6:1F:214:GLY:HA3	6:1F:220:THR:OG1	2.18	0.43
6:1F:247:ARG:HB2	6:1F:250:ASN:ND2	2.33	0.43
6:1F:337:MET:CE	6:1F:343:ILE:HG22	2.49	0.43
6:1F:349:ARG:NH1	6:1F:349:ARG:O	2.51	0.43
7:1G:13:VAL:HB	7:1G:33:VAL:HG21	2.00	0.43
7:1G:278:ARG:HE	7:1G:278:ARG:HB3	1.60	0.43
69:1L:701:3PE:H32	69:1L:701:3PE:C33	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:129:LEU:HD23	16:1P:160:PHE:CG	2.53	0.43
24:1Y:105:ARG:HD2	24:1Y:105:ARG:HA	1.61	0.43
69:1Y:205:3PE:C23	69:1Y:208:3PE:H261	2.48	0.43
70:1Y:207:PC1:H321	70:1Y:207:PC1:H352	1.73	0.43
69:1Y:210:3PE:H262	69:1Y:210:3PE:H232	1.62	0.43
29:1d:71:PHE:HD1	69:1d:203:3PE:H272	0.91	0.43
69:1d:201:3PE:H371	69:1d:201:3PE:H342	1.49	0.43
31:1f:21:VAL:CG2	69:1f:104:3PE:H3G1	2.47	0.43
38:1m:37:ALA:HB2	39:1n:149:ARG:NH1	2.34	0.43
69:1m:202:3PE:H351	69:1m:202:3PE:H381	1.75	0.43
40:1o:11:ASP:OD1	40:1o:13:SER:OG	2.34	0.43
42:1q:9:ARG:O	42:1q:13:GLN:HG3	2.19	0.43
42:1q:66:THR:HG23	42:1q:74:PHE:HD2	1.82	0.43
43:1r:42:VAL:HB	43:1r:46:HIS:CG	2.54	0.43
45:3A:358:LYS:HG2	45:3A:399:ILE:HG22	2.00	0.43
75:3A:501:CDL:H551	75:3A:501:CDL:H581	1.90	0.43
47:3C:364:VAL:O	47:3C:368:ILE:HG13	2.19	0.43
69:3C:508:3PE:H362	69:3C:508:3PE:H391	1.69	0.43
69:3C:512:3PE:H331	69:3C:513:3PE:H272	2.01	0.43
69:3G:103:3PE:H371	69:3G:108:3PE:H241	2.01	0.43
69:3G:104:3PE:H271	69:3G:104:3PE:C37	2.35	0.43
69:3G:104:3PE:H232	69:3G:104:3PE:H272	2.00	0.43
45:3N:442:PHE:HE1	45:3N:444:LEU:HD13	1.83	0.43
46:3O:307:PHE:H	49:3V:52:ARG:CD	2.32	0.43
47:3P:185:LEU:HD23	47:3P:185:LEU:HA	1.84	0.43
69:3P:515:3PE:H331	69:3P:515:3PE:H2A1	2.00	0.43
69:3P:516:3PE:H2F2	70:3T:102:PC1:C2G	2.49	0.43
48:3Q:204:MET:HG2	69:3R:302:3PE:H12	2.00	0.43
49:3R:168:LYS:HE3	49:3R:173:PRO:HG3	2.01	0.43
49:3R:224:PRO:HA	49:3R:237:PRO:HD3	2.01	0.43
54:3X:15:ARG:HH12	87:3X:102:PEK:P	2.41	0.43
70:3X:104:PC1:H2E2	70:3X:104:PC1:H2H1	1.87	0.43
69:3X:106:3PE:H351	69:3X:106:3PE:H321	1.68	0.43
55:4A:297:MET:O	55:4A:298:ASP:C	2.62	0.43
55:4A:372:TYR:N	55:4A:432:GLY:HA3	2.34	0.43
91:4A:608:PGV:H312	75:4B:302:CDL:C44	2.49	0.43
57:4C:145:THR:O	57:4C:149:HIS:ND1	2.29	0.43
58:4D:57:VAL:O	58:4D:61:ARG:HG2	2.18	0.43
60:4F:50:PRO:O	60:4F:56:ARG:NH1	2.46	0.43
91:4J:101:PGV:O13	91:4J:101:PGV:H222	2.18	0.43
4:1D:24:GLU:HG2	4:1D:25:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:143:GLU:HG3	4:1D:310:ILE:HB	2.01	0.42
5:1E:143:GLU:CD	6:1F:349:ARG:HH22	2.26	0.42
7:1G:160:ILE:HG13	7:1G:173:GLY:HA2	1.99	0.42
7:1G:359:ARG:HG2	7:1G:363:LEU:HD23	2.01	0.42
7:1G:478:ARG:HG3	7:1G:478:ARG:NH1	2.34	0.42
8:1H:277:TYR:HE2	70:1H:402:PC1:H272	1.82	0.42
10:1J:87:LYS:HD2	10:1J:90:PHE:CD2	2.46	0.42
69:1J:201:3PE:H3C1	69:1J:203:3PE:H292	2.02	0.42
12:1L:139:GLN:HG2	75:1L:704:CDL:H862	2.01	0.42
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	2.01	0.42
69:1L:709:3PE:H232	69:1L:709:3PE:O31	2.19	0.42
13:1M:201:MET:HG3	82:1Y:203:PGT:H422	1.99	0.42
15:1O:163:TYR:OH	15:1O:269:VAL:HG13	2.19	0.42
23:1X:15:GLN:HE21	23:1X:64:GLN:HG2	1.84	0.42
69:1Y:214:3PE:H3H1	75:3P:513:CDL:H712	2.01	0.42
69:1Y:216:3PE:H2H2	51:3T:50:PRO:HA	2.01	0.42
29:1d:53:VAL:H	69:1d:201:3PE:H111	1.84	0.42
70:1d:204:PC1:H12	70:1d:204:PC1:C31	2.49	0.42
47:3C:246:SER:HB2	69:3C:504:3PE:H121	2.01	0.42
49:3E:168:LYS:HD2	49:3E:168:LYS:HA	1.84	0.42
49:3E:218:THR:HG21	49:3E:256:LEU:HD23	2.00	0.42
49:3E:225:ILE:HG22	49:3E:226:ALA:N	2.34	0.42
51:3G:63:TRP:CZ2	69:3G:110:3PE:C2	3.02	0.42
45:3N:155:ALA:HA	45:3N:164:ALA:HB1	2.01	0.42
45:3N:158:PHE:O	45:3N:164:ALA:HB2	2.19	0.42
45:3N:344:ARG:HH12	45:3N:353:GLU:CD	2.27	0.42
47:3P:267:HIS:HD2	47:3P:269:LYS:HG2	1.84	0.42
75:3P:513:CDL:C76	75:3P:513:CDL:H651	2.49	0.42
48:3Q:27:ARG:O	48:3Q:31:GLN:HG3	2.18	0.42
48:3Q:41:HIS:CE1	48:3Q:111:PRO:HD2	2.51	0.42
48:3Q:149:PHE:CD2	48:3Q:151:PRO:HD3	2.54	0.42
49:3R:150:SER:HB3	49:3R:170:ARG:HA	2.00	0.42
49:3R:185:ASP:OD1	49:3R:185:ASP:N	2.52	0.42
50:3S:51:PRO:HD3	50:3S:93:TYR:OH	2.18	0.42
53:3W:31:PHE:CG	54:3X:48:ILE:HD11	2.54	0.42
54:3X:46:PRO:HD2	69:3X:101:3PE:H292	2.00	0.42
75:3X:103:CDL:HB62	75:3X:103:CDL:C54	2.49	0.42
75:3X:103:CDL:HB62	75:3X:103:CDL:C55	2.49	0.42
55:4A:71:MET:HB2	55:4A:72:PRO:HD3	2.01	0.42
55:4A:254:ILE:HD12	55:4A:341:ALA:HA	2.00	0.42
55:4A:346:PHE:HD2	91:4A:608:PGV:H281	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:4B:65:TRP:CD1	56:4B:65:TRP:C	2.97	0.42
58:4D:112:GLU:O	58:4D:116:VAL:HG23	2.19	0.42
62:4H:30:TRP:CE2	62:4H:34:LEU:HD11	2.53	0.42
2:1B:45:LEU:O	2:1B:47:PRO:HD3	2.19	0.42
2:1B:133:VAL:O	2:1B:135:GLY:N	2.52	0.42
7:1G:115:ASP:O	7:1G:119:GLN:HG3	2.18	0.42
7:1G:278:ARG:NH1	7:1G:568:GLU:OE2	2.51	0.42
7:1G:350:PRO:HB3	7:1G:464:THR:HA	2.00	0.42
8:1H:68:ILE:O	8:1H:72:ILE:HG23	2.18	0.42
8:1H:99:ASN:ND2	70:1H:403:PC1:H153	2.34	0.42
12:1L:467:ILE:HG21	69:1L:703:3PE:C37	2.48	0.42
69:1L:709:3PE:H342	69:1L:710:3PE:H272	2.01	0.42
69:1L:710:3PE:H222	33:1h:26:ARG:HD3	2.01	0.42
13:1M:9:THR:C	13:1M:11:LEU:H	2.27	0.42
14:1N:336:VAL:CG2	69:1d:203:3PE:H2H1	2.49	0.42
16:1P:82:ARG:HA	16:1P:82:ARG:HE	1.84	0.42
20:1T:64:ASP:CG	22:1W:37:ARG:HH12	2.27	0.42
21:1V:22:ARG:HH11	21:1V:25:ILE:HD11	1.83	0.42
31:1f:22:PHE:CE2	69:1f:104:3PE:H351	2.54	0.42
31:1f:31:ASP:OD1	31:1f:31:ASP:C	2.62	0.42
75:1g:201:CDL:H382	75:1g:201:CDL:C64	2.49	0.42
69:1m:205:3PE:H3A1	69:1m:205:3PE:C3E	2.47	0.42
40:1o:68:CYS:SG	40:1o:79:CYS:HB2	2.59	0.42
41:1p:5:ASP:OD1	41:1p:7:ASP:N	2.31	0.42
46:3B:95:LYS:NZ	49:3I:72:VAL:HB	2.34	0.42
46:3B:169:ARG:HG3	46:3B:240:ARG:HB2	2.01	0.42
69:3C:509:3PE:H3C2	69:3C:509:3PE:H382	2.00	0.42
48:3D:185:ASN:ND2	48:3D:188:ALA:H	2.17	0.42
48:3D:305:LEU:HB3	69:3G:101:3PE:H3B1	2.00	0.42
69:3D:503:3PE:H321	69:3D:503:3PE:H352	1.80	0.42
52:3H:50:GLU:C	52:3H:52:ILE:H	2.26	0.42
69:3P:516:3PE:H3E1	70:3T:102:PC1:H2D1	2.01	0.42
48:3Q:220:TYR:CE2	69:3T:103:3PE:H391	2.54	0.42
49:3R:168:LYS:HD3	49:3R:168:LYS:HA	1.83	0.42
75:3X:103:CDL:C21	69:3X:105:3PE:H3H2	2.48	0.42
55:4A:304:TYR:CE2	91:4N:101:PGV:H51	2.54	0.42
56:4B:104:TRP:CG	56:4B:203:ASN:HB2	2.54	0.42
57:4C:241:TYR:O	57:4C:245:VAL:HG13	2.20	0.42
91:4C:303:PGV:H341	91:4N:101:PGV:H321	2.01	0.42
61:4G:30:LEU:HD12	61:4G:30:LEU:HA	1.79	0.42
68:4N:57:LEU:HD23	68:4N:57:LEU:HA	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
91:4N:101:PGV:H52	91:4N:101:PGV:H21	1.79	0.42
1:1A:22:PHE:O	1:1A:23:TRP:CD1	2.73	0.42
2:1B:69:MET:HE2	2:1B:76:PHE:HD1	1.84	0.42
5:1E:51:LEU:HD22	5:1E:61:LEU:HD11	2.00	0.42
6:1F:43:TYR:CD1	6:1F:44:LYS:HG3	2.53	0.42
7:1G:436:ASN:OD1	7:1G:436:ASN:C	2.62	0.42
9:1I:57:LEU:HB2	42:1q:93:MET:HE3	2.02	0.42
12:1L:512:LYS:CD	64:4J:18:LEU:CD1	2.98	0.42
13:1M:15:THR:O	13:1M:93:LYS:HG2	2.18	0.42
15:1O:13:ARG:O	15:1O:16:ARG:HG2	2.20	0.42
15:1O:36:GLY:C	15:1O:40:ARG:NH1	2.77	0.42
15:1O:38:LEU:HD12	15:1O:38:LEU:HA	1.83	0.42
16:1P:245:ILE:HG23	16:1P:318:LEU:HD11	2.00	0.42
16:1P:268:ARG:HG2	16:1P:281:ARG:HD2	2.01	0.42
17:1Q:22:LEU:HD21	22:1W:78:VAL:HG13	2.00	0.42
19:1S:82:SER:O	19:1S:86:VAL:HG23	2.18	0.42
20:1T:34:SER:O	20:1T:73:PRO:HD3	2.19	0.42
70:1Y:206:PC1:H121	38:1m:81:PRO:CD	2.48	0.42
70:1Y:207:PC1:H271	69:1Y:209:3PE:H372	2.01	0.42
32:1g:90:ARG:NE	41:1p:100:GLU:OE1	2.49	0.42
69:1h:204:3PE:H232	69:1h:204:3PE:O13	2.19	0.42
36:1k:61:SER:OG	36:1k:62:PHE:N	2.52	0.42
37:1l:107:GLY:HA3	69:1l:203:3PE:H222	2.01	0.42
69:1m:201:3PE:H12	69:1m:201:3PE:C11	2.50	0.42
39:1n:55:ASP:CG	45:3N:221:GLY:O	2.62	0.42
40:1o:98:MET:HE2	40:1o:98:MET:HB3	1.93	0.42
69:1o:201:3PE:H232	69:1o:201:3PE:H331	2.00	0.42
43:1r:11:ARG:NH1	43:1r:20:GLN:HE21	2.17	0.42
45:3A:267:ASN:O	45:3A:271:GLN:HG3	2.19	0.42
45:3A:316:GLU:OE1	45:3A:316:GLU:N	2.52	0.42
69:3C:510:3PE:H122	69:3C:510:3PE:C2	2.40	0.42
69:3C:513:3PE:H321	69:3C:513:3PE:H351	1.90	0.42
48:3D:232:ARG:O	48:3D:232:ARG:HG3	2.14	0.42
49:3E:155:LYS:O	49:3E:270:LEU:HD22	2.20	0.42
50:3F:63:PRO:HG2	50:3F:66:LEU:HD12	2.02	0.42
45:3N:79:VAL:HG22	45:3N:112:LEU:HD23	2.01	0.42
45:3N:135:LEU:HD21	45:3N:174:VAL:CG2	2.50	0.42
46:3O:128:ALA:HA	46:3O:227:ARG:NH2	2.29	0.42
47:3P:95:PHE:CD1	69:3P:519:3PE:H3F1	2.54	0.42
69:3Q:504:3PE:H231	69:3Q:504:3PE:H332	2.00	0.42
55:4A:176:MET:HE2	55:4A:181:THR:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:336:PRO:HG3	55:4A:411:LYS:HG3	2.01	0.42
57:4C:182:TYR:CE1	61:4G:72:ASN:ND2	2.88	0.42
61:4G:64:ASP:OD1	61:4G:64:ASP:N	2.51	0.42
68:4N:38:LEU:C	68:4N:39:PHE:CG	2.98	0.42
70:1A:202:PC1:H221	70:1A:202:PC1:C32	2.49	0.42
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.44	0.42
69:1B:205:3PE:C35	75:1q:202:CDL:H572	2.50	0.42
4:1D:218:PHE:O	4:1D:222:ILE:HG13	2.19	0.42
6:1F:147:SER:O	6:1F:151:VAL:HG12	2.20	0.42
6:1F:429:ARG:HE	6:1F:429:ARG:HB2	1.66	0.42
7:1G:148:THR:HG22	7:1G:208:LEU:HD23	2.00	0.42
12:1L:137:LEU:HD12	12:1L:137:LEU:HA	1.81	0.42
12:1L:217:LEU:HD11	12:1L:277:THR:HB	2.00	0.42
12:1L:319:ILE:HG21	12:1L:399:VAL:HG23	2.02	0.42
13:1M:270:ILE:HD11	13:1M:395:LEU:O	2.19	0.42
15:1O:101:TYR:CE1	15:1O:128:ILE:HG23	2.51	0.42
16:1P:215:ILE:O	16:1P:218:ILE:HB	2.19	0.42
16:1P:325:ARG:HA	16:1P:325:ARG:HD2	1.84	0.42
17:1Q:49:VAL:O	17:1Q:49:VAL:HG22	2.19	0.42
20:1T:18:VAL:HG21	20:1T:54:MET:HG3	2.00	0.42
23:1X:110:VAL:HB	23:1X:116:TRP:HB2	2.00	0.42
24:1Y:79:VAL:HG11	69:1Y:214:3PE:C31	2.49	0.42
25:1Z:143:TYR:CE1	26:1a:48:MET:HE1	2.54	0.42
69:1d:201:3PE:H271	69:1d:201:3PE:H2A1	1.89	0.42
33:1h:36:VAL:HG23	70:1h:202:PC1:H2I3	2.00	0.42
33:1h:79:PHE:HD2	70:1h:203:PC1:H231	1.84	0.42
38:1m:92:PHE:HE1	69:1m:203:3PE:H372	1.70	0.42
40:1o:16:PRO:HB3	40:1o:104:GLU:HG2	2.01	0.42
40:1o:74:PRO:HB2	69:1o:201:3PE:H2C2	2.01	0.42
47:3C:106:SER:HA	47:3C:313:ARG:HH21	1.85	0.42
49:3E:219:HIS:HB2	49:3E:254:ALA:HB2	2.01	0.42
69:3G:102:3PE:H351	69:3G:102:3PE:H321	1.85	0.42
52:3H:53:GLU:O	52:3H:54:LYS:C	2.60	0.42
53:3J:5:THR:O	53:3J:9:ARG:HG3	2.18	0.42
46:3O:116:ILE:HD13	46:3O:116:ILE:HA	1.83	0.42
47:3P:114:ASN:HB3	70:3P:509:PC1:H252	2.00	0.42
47:3P:156:ILE:HD13	69:3P:507:3PE:H292	2.00	0.42
47:3P:186:PRO:HA	47:3P:189:ILE:HD12	2.01	0.42
47:3P:306:MET:CE	69:3P:514:3PE:C27	2.57	0.42
49:3R:121:THR:O	49:3R:125:VAL:HG23	2.19	0.42
49:3R:210:TRP:O	49:3R:265:PHE:CZ	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:3X:1:MET:HE3	69:3X:105:3PE:C24	2.50	0.42
69:3X:105:3PE:H342	69:3X:105:3PE:O21	2.19	0.42
69:3X:108:3PE:H322	61:4G:36:TRP:HE1	1.83	0.42
58:4D:63:LYS:HG2	58:4D:64:PHE:CZ	2.53	0.42
58:4D:120:THR:HG23	58:4D:134:PHE:HZ	1.84	0.42
1:1A:27:LEU:HD22	70:1A:202:PC1:H111	2.01	0.42
1:1A:48:ARG:NE	10:1J:78:MET:HA	2.30	0.42
2:1B:70:ASP:OD1	2:1B:75:VAL:HG12	2.19	0.42
4:1D:237:ASN:O	8:1H:284:GLN:NE2	2.47	0.42
4:1D:237:ASN:C	8:1H:284:GLN:HE22	2.28	0.42
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	2.01	0.42
6:1F:89:ARG:HB3	6:1F:218:CYS:HB3	2.01	0.42
6:1F:133:ALA:HB1	6:1F:176:PHE:HE1	1.83	0.42
6:1F:205:LEU:HD11	7:1G:50:GLY:O	2.19	0.42
6:1F:372:MET:HE3	6:1F:415:VAL:HG21	2.00	0.42
7:1G:596:ASP:O	7:1G:600:ILE:HG12	2.19	0.42
8:1H:296:LEU:HD13	70:1H:402:PC1:H351	2.01	0.42
12:1L:4:PHE:O	12:1L:8:THR:OG1	2.29	0.42
12:1L:149:ILE:HD12	12:1L:149:ILE:HA	1.76	0.42
12:1L:463:PHE:HE2	69:1k:101:3PE:H3I3	1.84	0.42
14:1N:41:ILE:HG23	14:1N:56:ALA:HB1	2.00	0.42
14:1N:88:LYS:HB2	14:1N:88:LYS:HE2	1.74	0.42
14:1N:226:THR:HG23	14:1N:229:SER:H	1.84	0.42
23:1X:168:PHE:CE1	75:1d:202:CDL:H141	2.54	0.42
24:1Y:27:ILE:CD1	69:1Y:208:3PE:C3I	2.97	0.42
24:1Y:111:ALA:O	70:1Y:207:PC1:H2C2	2.20	0.42
30:1e:29:PRO:HB3	33:1h:138:LYS:HG3	2.01	0.42
69:1e:201:3PE:H2C2	69:1e:201:3PE:H2F1	1.75	0.42
69:1m:203:3PE:C3A	69:1m:205:3PE:H3I1	2.49	0.42
42:1q:6:VAL:CG1	75:1q:201:CDL:OA9	2.65	0.42
47:3C:17:ALA:HA	47:3C:201:HIS:CE1	2.55	0.42
47:3C:197:LEU:HD23	47:3C:197:LEU:HA	1.92	0.42
69:3C:508:3PE:H321	69:3C:508:3PE:H271	2.02	0.42
69:3C:515:3PE:H11	69:3C:516:3PE:H31	2.02	0.42
50:3F:40:LYS:HA	50:3F:92:TRP:CD1	2.54	0.42
69:3J:104:3PE:H3A1	69:3J:104:3PE:H372	1.76	0.42
47:3P:150:LEU:HB3	47:3P:161:VAL:HG22	2.00	0.42
47:3P:284:ILE:H	47:3P:284:ILE:HG12	1.59	0.42
69:3P:505:3PE:H242	69:3P:518:3PE:O32	2.19	0.42
75:3P:513:CDL:H212	75:3P:513:CDL:H242	1.79	0.42
48:3Q:238:ARG:NH2	49:3R:83:ILE:HG22	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3Q:502:3PE:H321	69:3Q:502:3PE:H352	1.87	0.42
51:3T:28:HIS:HA	69:3T:103:3PE:H2G1	2.01	0.42
51:3T:32:LYS:HB2	51:3T:32:LYS:HE2	1.71	0.42
52:3U:24:CYS:O	52:3U:27:ILE:HG12	2.20	0.42
55:4A:202:LEU:HD22	55:4A:238:PHE:CE2	2.54	0.42
55:4A:361:SER:HB3	56:4B:84:LEU:HD22	2.02	0.42
57:4C:31:LEU:HD11	87:4G:103:PEK:H302	2.01	0.42
58:4D:55:GLU:HA	58:4D:58:GLU:HG2	2.01	0.42
64:4J:52:TRP:O	64:4J:57:HIS:ND1	2.52	0.42
4:1D:275:TYR:CZ	4:1D:367:ILE:HB	2.55	0.42
4:1D:371:LYS:NZ	4:1D:422:ASP:HB2	2.35	0.42
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.93	0.42
5:1E:163:ASP:OD2	5:1E:186:PRO:HB3	2.20	0.42
5:1E:192:SER:OG	5:1E:193:CYS:N	2.52	0.42
7:1G:7:ASN:OD1	7:1G:7:ASN:N	2.49	0.42
7:1G:146:VAL:HG12	7:1G:200:ILE:HD11	2.01	0.42
10:1J:103:MET:HB2	10:1J:103:MET:HE3	1.76	0.42
12:1L:50:PRO:HA	12:1L:53:MET:HG3	2.01	0.42
12:1L:583:LEU:HB2	12:1L:586:LEU:HG	2.01	0.42
69:1L:712:3PE:H362	69:1L:712:3PE:H392	1.51	0.42
14:1N:95:MET:HE2	14:1N:149:ILE:HA	2.01	0.42
14:1N:129:LEU:CD1	75:1N:402:CDL:C54	2.97	0.42
14:1N:317:PHE:CZ	15:1O:106:LEU:HD11	2.47	0.42
20:1U:78:ASP:HB3	34:1i:15:ARG:NH1	2.34	0.42
24:1Y:6:HIS:O	24:1Y:10:ASP:CG	2.62	0.42
24:1Y:72:THR:HB	24:1Y:92:GLY:HA2	2.01	0.42
70:1Y:207:PC1:H281	69:1Y:209:3PE:H372	2.01	0.42
69:1Y:215:3PE:C3C	70:3T:102:PC1:H3C2	2.45	0.42
29:1d:28:ASP:HA	29:1d:29:PRO:HD3	1.97	0.42
30:1e:59:PHE:O	30:1e:63:VAL:HG23	2.20	0.42
75:3A:501:CDL:OB4	69:3A:502:3PE:H122	2.20	0.42
47:3C:231:GLY:CA	75:3D:504:CDL:H732	2.45	0.42
69:3C:512:3PE:H392	69:3C:512:3PE:H361	1.89	0.42
48:3D:96:PRO:HG2	52:3H:91:ASP:HB3	2.01	0.42
49:3E:181:LYS:HA	49:3E:181:LYS:HD3	1.80	0.42
45:3N:12:PRO:HG2	45:3N:28:GLU:OE2	2.19	0.42
69:3N:501:3PE:H3B2	75:3N:502:CDL:H352	2.00	0.42
46:3O:46:ARG:HG2	46:3O:379:LEU:HD22	2.02	0.42
46:3O:51:ILE:HG23	46:3O:204:MET:HG2	2.02	0.42
46:3O:152:PHE:C	46:3O:154:ASN:N	2.73	0.42
46:3O:203:ARG:NH1	46:3O:232:LEU:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3R:159:ILE:HG21	49:3R:176:VAL:HG12	2.01	0.42
69:3X:101:3PE:C2B	69:3X:108:3PE:H2F2	2.31	0.42
69:3X:108:3PE:H332	69:4G:104:3PE:H331	2.02	0.42
55:4A:507:GLU:HA	57:4C:5:THR:HB	2.00	0.42
56:4B:74:ILE:HG13	56:4B:75:LEU:N	2.35	0.42
62:4H:57:ARG:HA	62:4H:60:TYR:CE2	2.54	0.42
63:4I:58:LYS:HB3	63:4I:58:LYS:HE3	1.84	0.42
68:4N:3:ARG:NH1	68:4N:4:GLN:HB2	2.34	0.42
69:1A:203:3PE:H2D2	69:1A:203:3PE:C29	2.49	0.42
69:1A:203:3PE:H342	69:1A:203:3PE:H371	1.82	0.42
2:1B:96:MET:HB2	4:1D:82:LEU:HD22	2.01	0.42
4:1D:136:TRP:HA	4:1D:139:VAL:HG12	2.02	0.42
4:1D:247:ALA:HA	4:1D:265:ILE:HD11	2.01	0.42
4:1D:261:ARG:HG2	4:1D:287:ILE:HD13	2.02	0.42
7:1G:315:VAL:HG23	7:1G:521:VAL:HB	2.00	0.42
8:1H:179:TRP:CG	8:1H:180:PRO:CD	3.03	0.42
8:1H:264:LEU:HD13	26:1a:9:ILE:CG2	2.50	0.42
10:1J:46:ASN:HD21	25:1Z:142:TRP:HE1	1.67	0.42
11:1K:37:MET:O	11:1K:41:PHE:N	2.46	0.42
12:1L:467:ILE:CD1	69:1L:703:3PE:H322	2.48	0.42
13:1M:294:MET:HE1	13:1M:316:MET:HG2	2.01	0.42
13:1M:318:ALA:HB1	13:1M:374:ASN:CG	2.44	0.42
21:1V:97:LYS:HA	21:1V:97:LYS:HD3	1.65	0.42
22:1W:62:LYS:HA	22:1W:62:LYS:HD3	1.75	0.42
22:1W:88:MET:O	22:1W:92:GLU:HG3	2.19	0.42
24:1Y:28:GLY:HA3	69:1Y:208:3PE:H382	2.01	0.42
24:1Y:120:THR:OG1	70:1Y:206:PC1:H3D2	2.19	0.42
75:1Y:217:CDL:H871	75:1Y:217:CDL:H841	1.80	0.42
69:1d:206:3PE:H351	69:1f:104:3PE:H271	2.02	0.42
30:1e:62:PHE:CE1	30:1e:66:LEU:HD21	2.54	0.42
30:1e:83:ASP:OD1	30:1e:84:LYS:N	2.53	0.42
75:1g:201:CDL:C65	33:1h:35:PRO:HG2	2.47	0.42
33:1h:113:LEU:HD12	33:1h:113:LEU:HA	1.83	0.42
43:1r:11:ARG:HH11	43:1r:20:GLN:HG2	1.84	0.42
46:3B:223:PHE:CD1	46:3B:223:PHE:N	2.87	0.42
48:3D:128:CYS:SG	86:3D:501:HEC:HBC3	2.60	0.42
69:3D:503:3PE:C23	69:3G:102:3PE:H361	2.50	0.42
49:3E:177:ARG:HD2	49:3E:179:ARG:HG2	2.01	0.42
47:3P:46:LEU:CD2	69:3R:302:3PE:H2D2	2.49	0.42
50:3S:51:PRO:CG	50:3S:54:LEU:HD12	2.49	0.42
70:3T:102:PC1:H322	70:3T:102:PC1:C25	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:181:THR:O	55:4A:270:TYR:OH	2.33	0.42
56:4B:91:ASN:O	56:4B:93:PRO:HD3	2.19	0.42
68:4N:50:ASN:OD1	68:4N:56:LYS:HD3	2.19	0.42
4:1D:115:GLU:HG3	4:1D:194:ILE:HB	2.01	0.42
5:1E:196:ALA:HB3	6:1F:264:HIS:CE1	2.55	0.42
6:1F:365:CYS:SG	6:1F:407:LEU:HD22	2.59	0.42
7:1G:335:LEU:O	7:1G:340:SER:OG	2.26	0.42
8:1H:173:TRP:NE1	70:1H:404:PC1:C12	2.82	0.42
9:1I:152:GLU:H	9:1I:152:GLU:HG2	1.68	0.42
10:1J:13:PHE:CZ	10:1J:17:PHE:CE1	3.08	0.42
10:1J:88:THR:HG23	69:1J:203:3PE:H232	2.01	0.42
11:1K:5:TYR:O	11:1K:9:ILE:HG13	2.19	0.42
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.20	0.42
69:1L:709:3PE:H112	33:1h:22:LEU:HB2	2.02	0.42
69:1M:502:3PE:H342	69:1m:205:3PE:H332	2.01	0.42
14:1N:247:THR:O	14:1N:251:MET:HG3	2.19	0.42
14:1N:269:GLU:OE2	14:1N:270:MET:HG3	2.19	0.42
15:1O:137:ALA:C	15:1O:139:TYR:N	2.77	0.42
16:1P:46:ILE:HD12	18:1R:26:VAL:HG21	2.01	0.42
16:1P:244:TYR:O	16:1P:248:VAL:HG23	2.20	0.42
17:1Q:50:ASN:O	17:1Q:53:LYS:HG3	2.20	0.42
17:1Q:106:GLU:H	17:1Q:106:GLU:HG2	1.75	0.42
21:1V:8:THR:OG1	21:1V:13:LEU:O	2.26	0.42
69:1Y:209:3PE:H262	69:1Y:213:3PE:H242	2.02	0.42
69:1Y:215:3PE:H382	69:1Y:215:3PE:H3B1	1.75	0.42
26:1a:27:HIS:O	26:1a:31:ASN:ND2	2.42	0.42
29:1d:33:TYR:CE1	75:1d:202:CDL:C41	3.03	0.42
69:1d:201:3PE:H351	69:1d:201:3PE:H322	1.23	0.42
32:1g:90:ARG:HA	32:1g:90:ARG:HD3	1.87	0.42
33:1h:94:LEU:HD23	33:1h:94:LEU:HA	1.91	0.42
45:3A:242:ARG:O	51:3G:16:ILE:HA	2.19	0.42
45:3A:445:ARG:NH1	75:3A:501:CDL:HB21	2.34	0.42
69:3A:502:3PE:H221	69:3A:502:3PE:H2	1.70	0.42
47:3C:75:TYR:O	47:3C:79:ILE:HG13	2.20	0.42
49:3E:163:LYS:HE2	49:3E:165:MET:HE1	2.01	0.42
49:3E:190:VAL:CG2	49:3E:250:ARG:HD3	2.49	0.42
49:3I:32:ALA:N	49:3I:71:ASN:HB3	2.35	0.42
69:3N:501:3PE:H2A1	75:3N:502:CDL:H551	2.01	0.42
69:3N:501:3PE:C3B	47:3P:14:ILE:CD1	2.90	0.42
46:3O:25:GLU:O	46:3O:36:ALA:HA	2.20	0.42
46:3O:33:LEU:HB2	46:3O:201:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3O:78:LYS:HG3	46:3O:129:ALA:O	2.19	0.42
69:3Q:504:3PE:H2	69:3Q:504:3PE:H332	2.02	0.42
50:3S:32:MET:HE2	50:3S:61:ARG:NH2	2.35	0.42
50:3S:91:GLU:N	50:3S:92:PRO:HD2	2.34	0.42
75:3X:103:CDL:PB2	75:3X:103:CDL:O1	2.78	0.42
69:3Y:101:3PE:H2I3	69:3Y:101:3PE:H2F2	1.81	0.42
55:4A:426:PHE:HB3	75:4B:302:CDL:H851	2.02	0.42
57:4C:22:LEU:O	57:4C:26:LEU:HG	2.20	0.42
57:4C:86:PHE:CE2	91:4C:305:PGV:H281	2.54	0.42
91:4C:303:PGV:O02	91:4C:303:PGV:H011	2.19	0.42
63:4I:73:LYS:HA	63:4I:73:LYS:HD2	1.80	0.42
68:4N:46:ASP:HB3	68:4N:49:ASN:O	2.18	0.42
1:1A:26:GLN:C	1:1A:27:LEU:HD12	2.45	0.42
1:1A:92:LEU:HD13	27:1b:29:ILE:HG12	2.01	0.42
4:1D:52:GLY:H	4:1D:53:PRO:CD	2.26	0.42
5:1E:105:THR:HG21	5:1E:144:CYS:H	1.84	0.42
70:1H:403:PC1:H2A1	10:1J:42:GLY:HA2	2.00	0.42
11:1K:2:PRO:HD2	11:1K:5:TYR:CD2	2.54	0.42
12:1L:100:ILE:O	12:1L:104:SER:OG	2.37	0.42
12:1L:416:THR:O	12:1L:419:THR:OG1	2.35	0.42
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.55	0.42
12:1L:524:ASN:ND2	39:1n:76:PRO:HB2	2.30	0.42
12:1L:570:GLN:CB	69:1L:705:3PE:H241	2.37	0.42
24:1Y:139:LYS:NZ	33:1h:112:ARG:HD3	2.35	0.42
69:1Y:211:3PE:H282	69:1Y:211:3PE:H251	1.90	0.42
37:1l:40:ASP:OD1	37:1l:40:ASP:N	2.52	0.42
43:1r:4:THR:O	43:1r:5:ARG:C	2.63	0.42
45:3A:49:ASN:C	45:3A:165:GLN:HE22	2.27	0.42
45:3A:192:ALA:N	45:3A:219:LEU:HD22	2.35	0.42
75:3A:501:CDL:H762	75:3A:501:CDL:H791	1.90	0.42
47:3C:8:HIS:CG	47:3C:11:MET:HE3	2.55	0.42
48:3D:326:TYR:CE1	51:3G:14:HIS:HB2	2.55	0.42
49:3E:95:GLU:CD	49:3E:95:GLU:H	2.28	0.42
49:3E:254:ALA:O	49:3E:256:LEU:N	2.53	0.42
49:3E:256:LEU:HG	49:3E:257:ASN:N	2.35	0.42
49:3E:270:LEU:C	49:3E:271:VAL:HG13	2.45	0.42
69:3G:104:3PE:H231	69:3G:104:3PE:H331	2.02	0.42
45:3N:42:ASP:CG	45:3N:384:LEU:HD22	2.45	0.42
46:3O:217:LYS:O	46:3O:221:GLU:HG2	2.18	0.42
47:3P:249:LEU:CD1	69:3P:520:3PE:C2	2.74	0.42
47:3P:350:ILE:HD11	51:3T:61:TRP:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3P:510:3PE:H392	69:3P:510:3PE:H361	1.70	0.42
69:3P:517:3PE:H32	69:3P:518:3PE:H241	2.02	0.42
48:3Q:110:PRO:HA	48:3Q:111:PRO:HD3	1.90	0.42
49:3R:167:PHE:HB3	49:3R:169:TRP:CE2	2.55	0.42
49:3R:180:THR:O	49:3R:182:LYS:HE2	2.19	0.42
49:3R:182:LYS:HD3	49:3R:182:LYS:N	2.34	0.42
49:3R:272:ILE:O	49:3R:273:VAL:C	2.62	0.42
52:3U:21:ARG:O	52:3U:25:GLU:N	2.51	0.42
54:3Y:15:ARG:HA	54:3Y:18:ILE:HD12	2.02	0.42
55:4A:510:TYR:CE1	60:4F:49:VAL:HG12	2.55	0.42
57:4C:45:LEU:HD11	64:4J:38:LEU:HG	2.01	0.42
58:4D:129:ALA:HB3	58:4D:134:PHE:H	1.85	0.42
65:4K:48:VAL:O	65:4K:50:PRO:HD3	2.19	0.42
1:1A:27:LEU:CG	8:1H:59:GLU:HG3	2.37	0.42
69:1B:204:3PE:H2A1	69:1B:204:3PE:H271	1.72	0.42
3:1C:35:LYS:HD3	3:1C:36:TYR:CZ	2.54	0.42
6:1F:137:TYR:HB3	6:1F:192:LEU:HD11	2.02	0.42
6:1F:186:CYS:SG	6:1F:195:SER:HB2	2.60	0.42
7:1G:110:GLN:CG	7:1G:114:CYS:HA	2.34	0.42
7:1G:203:CYS:HG	71:1G:802:SF4:FE4	1.32	0.42
7:1G:379:LEU:HD23	7:1G:452:VAL:HB	2.02	0.42
7:1G:582:GLN:HB3	7:1G:633:TYR:CE1	2.55	0.42
9:1I:54:LYS:HD3	42:1q:91:HIS:NE2	2.35	0.42
10:1J:150:GLY:O	10:1J:154:VAL:HG23	2.20	0.42
12:1L:184:LEU:HD12	13:1M:393:ILE:HG13	2.02	0.42
12:1L:558:LEU:HD23	12:1L:558:LEU:HA	1.87	0.42
12:1L:573:MET:HG2	14:1N:167:TRP:CH2	2.55	0.42
69:1L:711:3PE:H331	69:1M:502:3PE:H282	2.01	0.42
13:1M:1:FME:HG3	13:1M:52:PHE:CE2	2.55	0.42
14:1N:65:THR:O	14:1N:69:MET:HG3	2.20	0.42
20:1T:54:MET:SD	20:1T:76:ILE:HG21	2.60	0.42
20:1U:16:LEU:HA	20:1U:19:LEU:HD23	2.02	0.42
20:1U:25:ILE:HD11	20:1U:42:LEU:HD11	2.01	0.42
20:1U:57:GLU:OE1	35:1j:11:TYR:OH	2.38	0.42
23:1X:7:PRO:HB2	23:1X:12:LEU:HD23	2.02	0.42
24:1Y:45:PRO:HG2	24:1Y:51:GLY:HA3	2.02	0.42
69:1d:201:3PE:H232	69:1d:201:3PE:H261	1.85	0.42
75:1g:201:CDL:H362	75:1g:201:CDL:H332	1.76	0.42
38:1m:39:ARG:HB2	38:1m:39:ARG:HH11	1.84	0.42
40:1o:33:ARG:HA	40:1o:33:ARG:HD2	1.77	0.42
42:1q:27:LEU:O	42:1q:31:ASN:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:214:LYS:HB2	45:3A:214:LYS:NZ	2.35	0.42
45:3A:255:ILE:HG23	45:3A:342:TRP:HH2	1.84	0.42
69:3A:502:3PE:H291	69:3A:502:3PE:H261	1.91	0.42
48:3D:163:ASN:CG	48:3D:164:GLU:N	2.78	0.42
49:3E:155:LYS:CD	49:3E:176:VAL:HG11	2.50	0.42
49:3E:225:ILE:HG12	49:3E:237:PRO:CD	2.50	0.42
50:3F:30:LYS:HE2	50:3F:30:LYS:HB3	1.70	0.42
45:3N:206:ARG:HH21	45:3N:209:LEU:HB3	1.85	0.42
69:3N:503:3PE:H291	69:3N:503:3PE:H261	1.74	0.42
48:3Q:91:PHE:HA	48:3Q:92:PRO:HD3	1.95	0.42
49:3R:93:ARG:HD3	69:3R:305:3PE:C12	2.48	0.42
49:3R:187:GLU:HG2	49:3R:246:SER:H	1.85	0.42
49:3R:212:ILE:HD13	49:3R:265:PHE:CZ	2.55	0.42
49:3R:271:VAL:HB	49:3R:273:VAL:HG23	2.02	0.42
69:3X:107:3PE:C1	69:3X:107:3PE:H242	2.50	0.42
55:4A:418:PHE:CZ	91:4A:608:PGV:H141	2.55	0.42
55:4A:477:ALA:HB1	66:4L:18:LYS:HZ1	1.85	0.42
91:4A:609:PGV:H21	66:4L:12:PRO:HB2	2.02	0.42
56:4B:97:VAL:HB	56:4B:152:MET:HE2	2.01	0.42
57:4C:90:GLU:OE1	91:4C:305:PGV:H321	2.20	0.42
70:1B:203:PC1:H3D1	69:1B:204:3PE:H3H2	2.02	0.41
3:1C:192:GLN:HB2	17:1Q:72:TRP:CD1	2.55	0.41
5:1E:202:LEU:HD12	6:1F:26:TYR:HB2	2.01	0.41
6:1F:371:TRP:CE2	7:1G:130:PHE:HD1	2.37	0.41
10:1J:7:PHE:O	10:1J:8:ILE:C	2.63	0.41
10:1J:167:VAL:HG13	14:1N:42:PRO:HG3	2.02	0.41
12:1L:34:ASN:O	12:1L:38:THR:OG1	2.38	0.41
12:1L:384:PRO:HA	12:1L:389:PHE:CD1	2.55	0.41
12:1L:573:MET:HG2	14:1N:167:TRP:CE2	2.55	0.41
13:1M:75:LEU:HD13	13:1M:440:HIS:CE1	2.55	0.41
70:1M:501:PC1:H143	70:1M:501:PC1:H112	1.68	0.41
24:1Y:98:LEU:CD1	69:1Y:212:3PE:H2F2	2.49	0.41
29:1d:62:LEU:HD23	29:1d:62:LEU:HA	1.93	0.41
29:1d:90:MET:O	29:1d:94:VAL:HG23	2.20	0.41
69:1d:201:3PE:H362	69:1d:201:3PE:H391	1.19	0.41
32:1g:63:PHE:O	32:1g:68:ILE:HG13	2.20	0.41
75:1g:201:CDL:H771	33:1h:35:PRO:HD3	2.00	0.41
38:1m:82:THR:H	38:1m:85:THR:HG1	1.66	0.41
44:1s:42:GLN:CD	44:1s:42:GLN:H	2.28	0.41
45:3A:248:LEU:HB2	45:3A:427:PRO:HD3	2.02	0.41
46:3B:382:VAL:HG22	46:3B:392:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:3C:285:PRO:CG	69:3C:512:3PE:H222	2.50	0.41
47:3C:287:LYS:HB2	69:3C:513:3PE:N	2.33	0.41
69:3C:507:3PE:H331	69:3C:507:3PE:H362	1.82	0.41
48:3D:314:HIS:NE2	51:3G:22:PRO:HB2	2.34	0.41
49:3E:187:GLU:OE1	49:3E:245:ALA:HB3	2.20	0.41
51:3G:63:TRP:CH2	69:3G:111:3PE:O31	2.73	0.41
69:3G:103:3PE:H112	69:3G:104:3PE:HN2	1.85	0.41
69:3G:110:3PE:H282	69:3G:110:3PE:H2B1	1.88	0.41
75:3N:502:CDL:H592	75:3N:502:CDL:H562	1.72	0.41
47:3P:304:MET:H	47:3P:304:MET:HG2	1.67	0.41
69:3P:508:3PE:H391	75:3P:513:CDL:H372	2.02	0.41
48:3Q:12:TRP:CD1	48:3Q:15:ARG:HH21	2.39	0.41
49:3R:186:GLN:O	49:3R:190:VAL:HG23	2.19	0.41
69:3W:103:3PE:H2G1	69:3W:103:3PE:H3C2	2.02	0.41
54:3Y:33:VAL:HB	69:3Y:105:3PE:H2H1	2.01	0.41
54:3Y:49:ASN:HD22	69:3Y:102:3PE:H11	1.85	0.41
55:4A:218:THR:HG21	61:4G:55:ILE:HD13	2.01	0.41
58:4D:18:ASP:OD2	58:4D:66:GLU:HB2	2.20	0.41
58:4D:53:MET:HE3	59:4E:104:LEU:HD23	2.02	0.41
58:4D:121:LYS:HB2	65:4K:50:PRO:HB3	2.02	0.41
59:4E:49:ASP:O	59:4E:53:ARG:HG3	2.20	0.41
60:4F:7:PRO:HG3	60:4F:12:GLN:NE2	2.35	0.41
66:4L:18:LYS:H	66:4L:18:LYS:HG3	1.71	0.41
68:4N:32:TYR:O	68:4N:34:THR:N	2.45	0.41
2:1B:50:PHE:CE1	2:1B:103:VAL:HG21	2.55	0.41
70:1B:203:PC1:H332	70:1B:203:PC1:H361	1.84	0.41
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.53	0.41
4:1D:405:MET:HE3	4:1D:405:MET:HB3	1.88	0.41
6:1F:394:GLU:OE2	43:1r:50:ASN:N	2.42	0.41
7:1G:24:THR:O	7:1G:73:VAL:HG22	2.19	0.41
8:1H:30:TYR:CD2	26:1a:5:ILE:HD11	2.55	0.41
8:1H:124:ASN:C	8:1H:126:LYS:H	2.28	0.41
10:1J:21:SER:HB3	11:1K:14:ILE:HD13	2.01	0.41
12:1L:174:TYR:OH	12:1L:534:HIS:NE2	2.48	0.41
12:1L:407:TRP:CE3	37:1l:115:MET:HE2	2.56	0.41
14:1N:102:LEU:HD13	14:1N:142:LEU:HG	2.02	0.41
14:1N:207:ILE:O	14:1N:211:MET:HG3	2.20	0.41
15:1O:165:PRO:HB3	15:1O:217:LYS:NZ	2.35	0.41
16:1P:208:VAL:O	16:1P:212:LYS:HG3	2.19	0.41
18:1R:13:HIS:HD1	18:1R:13:HIS:H	1.68	0.41
20:1U:51:ILE:HG21	20:1U:67:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:1Y:217:CDL:H112	75:1Y:217:CDL:C15	2.50	0.41
26:1a:41:PHE:O	26:1a:42:SER:C	2.62	0.41
69:1d:206:3PE:H2B1	69:1f:104:3PE:H2C2	2.00	0.41
40:1o:43:GLN:NE2	40:1o:47:ASP:OD2	2.53	0.41
45:3A:280:TYR:O	45:3A:306:SER:HA	2.19	0.41
69:3A:503:3PE:H3A2	69:3A:503:3PE:H3D2	1.74	0.41
46:3B:366:ALA:HB1	46:3B:370:MET:HE3	2.02	0.41
47:3C:374:ASN:O	47:3C:379:TRP:HD1	2.03	0.41
69:3C:513:3PE:H281	69:3C:513:3PE:H251	1.89	0.41
69:3C:515:3PE:H2B2	69:3C:515:3PE:H281	1.55	0.41
48:3D:101:SER:O	48:3D:107:SER:HB3	2.19	0.41
49:3E:170:ARG:HD3	47:3P:168:PHE:CB	2.50	0.41
69:3N:501:3PE:H251	69:3N:501:3PE:H221	1.81	0.41
69:3N:503:3PE:H261	69:3N:503:3PE:H2B2	2.03	0.41
47:3P:356:ILE:HG12	69:3P:517:3PE:H351	2.02	0.41
69:3P:504:3PE:H352	69:3P:504:3PE:H322	1.78	0.41
69:3P:520:3PE:H3A1	69:3Q:504:3PE:H361	2.02	0.41
48:3Q:216:LEU:HB2	48:3Q:217:PRO:HD3	2.03	0.41
69:3T:103:3PE:H2I1	69:3T:103:3PE:C32	2.47	0.41
70:3X:104:PC1:H31	70:3X:104:PC1:H112	2.01	0.41
69:3X:108:3PE:H241	69:3X:108:3PE:O22	2.20	0.41
54:3Y:18:ILE:HG22	69:3Y:101:3PE:H232	2.02	0.41
69:3Y:107:3PE:H11	69:3Y:107:3PE:C11	2.50	0.41
55:4A:44:PRO:HD3	55:4A:448:THR:HG23	2.02	0.41
55:4A:379:TYR:HA	55:4A:383:MET:HG3	2.01	0.41
56:4B:32:PHE:HE2	75:4B:302:CDL:OA9	2.02	0.41
57:4C:251:PHE:C	57:4C:253:TYR:N	2.76	0.41
91:4C:304:PGV:H31	61:4G:70:PHE:CE2	2.51	0.41
62:4H:43:MET:HE2	68:4N:82:PHE:HB3	2.01	0.41
62:4H:75:ARG:HA	62:4H:78:GLU:HG2	2.02	0.41
91:4K:101:PGV:H011	91:4K:101:PGV:O12	2.20	0.41
66:4L:23:ALA:HA	66:4L:26:THR:HG22	2.02	0.41
68:4N:13:PRO:HA	68:4N:16:ILE:HD12	2.02	0.41
1:1A:23:TRP:CZ3	70:1P:502:PC1:H231	2.54	0.41
70:1B:203:PC1:H271	8:1H:46:LEU:HD11	2.02	0.41
7:1G:427:LYS:HE2	7:1G:427:LYS:HB2	1.63	0.41
8:1H:115:SER:O	8:1H:119:SER:HB3	2.20	0.41
70:1H:404:PC1:H132	70:1H:404:PC1:H112	1.56	0.41
10:1J:61:LEU:HD12	10:1J:65:LEU:HD12	2.02	0.41
10:1J:132:ASP:OD1	26:1a:42:SER:OG	2.34	0.41
11:1K:90:VAL:HA	11:1K:93:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:23:ASN:HB3	69:1L:709:3PE:P	2.58	0.41
12:1L:124:PHE:CE2	12:1L:247:LEU:HG	2.54	0.41
12:1L:464:ALA:HA	69:1L:703:3PE:H2A2	2.01	0.41
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	2.02	0.41
14:1N:40:MET:O	14:1N:44:LEU:HG	2.20	0.41
20:1U:45:LEU:HD23	39:1n:44:ARG:NH1	2.35	0.41
24:1Y:22:TYR:CD1	75:1Y:217:CDL:C47	3.03	0.41
24:1Y:95:ALA:CB	70:1Y:207:PC1:C3C	2.95	0.41
69:1Y:215:3PE:C2D	70:3T:102:PC1:H3A1	2.50	0.41
75:1g:201:CDL:H621	75:1g:201:CDL:C76	2.50	0.41
34:1i:105:PRO:HA	34:1i:116:ILE:HB	2.01	0.41
69:1m:203:3PE:C3D	69:1m:205:3PE:H2I1	2.51	0.41
45:3A:390:ILE:HG23	45:3A:394:GLU:CD	2.45	0.41
45:3A:430:GLN:HG2	45:3A:430:GLN:O	2.20	0.41
69:3A:502:3PE:H3G1	69:3E:302:3PE:H2E1	2.02	0.41
47:3C:156:ILE:HD13	70:3X:104:PC1:H271	2.02	0.41
47:3C:224:TYR:O	47:3C:228:ASP:HB2	2.20	0.41
47:3C:289:GLY:O	69:3C:512:3PE:H351	2.20	0.41
47:3C:366:MET:HB2	47:3C:367:PRO:HD3	2.01	0.41
69:3C:507:3PE:H352	69:3C:507:3PE:C2A	2.50	0.41
69:3C:511:3PE:H332	69:3C:512:3PE:H262	2.02	0.41
48:3D:102:HIS:O	48:3D:291:LYS:NZ	2.53	0.41
48:3D:198:PRO:HA	48:3D:199:PRO:HD3	1.88	0.41
49:3E:133:VAL:HG22	69:3E:303:3PE:H2E2	2.02	0.41
49:3E:182:LYS:HE2	49:3E:182:LYS:HB2	1.83	0.41
49:3E:191:GLU:HB3	49:3E:194:GLN:CG	2.50	0.41
49:3E:252:GLY:HA2	49:3E:253:PRO:HD3	1.91	0.41
53:3J:22:ALA:HB1	70:3J:106:PC1:H272	2.02	0.41
69:3P:518:3PE:H322	69:3P:518:3PE:C26	2.50	0.41
69:3W:103:3PE:H3I2	69:3W:103:3PE:H3F2	1.86	0.41
55:4A:115:SER:HB2	55:4A:145:LEU:HB2	2.01	0.41
55:4A:233:HIS:HB3	57:4C:99:TRP:CZ2	2.55	0.41
55:4A:290:HIS:CG	88:4A:602:HEA:HMA	2.55	0.41
55:4A:295:VAL:HG23	55:4A:297:MET:HG3	2.02	0.41
57:4C:117:PRO:HA	57:4C:118:PRO:HD3	1.96	0.41
91:4C:303:PGV:H272	91:4C:303:PGV:C7	2.44	0.41
4:1D:228:MET:HE1	9:1I:36:MET:HB3	2.02	0.41
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	2.02	0.41
7:1G:35:MET:SD	7:1G:81:THR:OG1	2.76	0.41
7:1G:119:GLN:O	7:1G:123:PHE:N	2.45	0.41
7:1G:156:CYS:O	71:1G:802:SF4:S4	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:415:LEU:O	7:1G:416:THR:OG1	2.33	0.41
9:1I:143:THR:OG1	9:1I:146:GLU:HG3	2.20	0.41
10:1J:17:PHE:CE2	11:1K:11:ALA:HB1	2.55	0.41
11:1K:42:ILE:O	11:1K:46:LEU:HD13	2.20	0.41
12:1L:146:GLY:HA2	75:1L:704:CDL:C76	2.50	0.41
12:1L:604:TYR:CD2	14:1N:153:LEU:HD13	2.56	0.41
13:1M:423:ILE:HG12	38:1m:58:VAL:HG12	2.03	0.41
14:1N:107:GLY:HA2	14:1N:111:PHE:O	2.21	0.41
14:1N:129:LEU:HD12	14:1N:129:LEU:HA	1.85	0.41
15:1O:35:LYS:HE3	15:1O:126:ARG:HG3	2.01	0.41
15:1O:100:LEU:HD11	77:1O:401:GTP:O6	2.20	0.41
16:1P:35:VAL:HG22	16:1P:45:VAL:HG11	2.02	0.41
16:1P:260:HIS:O	16:1P:264:ARG:HG3	2.21	0.41
20:1U:15:VAL:O	20:1U:19:LEU:HD22	2.21	0.41
22:1W:87:LYS:HE2	22:1W:87:LYS:HB2	1.68	0.41
75:1d:202:CDL:H542	75:1d:202:CDL:H572	1.77	0.41
69:1f:103:3PE:C2F	69:1g:202:3PE:H3I2	2.50	0.41
69:1f:104:3PE:H332	69:1f:104:3PE:C24	2.41	0.41
33:1h:38:ILE:O	33:1h:41:THR:OG1	2.31	0.41
69:1m:205:3PE:H231	69:1m:205:3PE:H261	1.85	0.41
75:3A:501:CDL:H142	69:3A:503:3PE:H352	2.02	0.41
75:3A:501:CDL:C75	69:3A:502:3PE:H2D2	2.44	0.41
46:3B:249:GLY:O	46:3B:250:ASP:O	2.38	0.41
46:3B:252:LEU:HD12	46:3B:252:LEU:HA	1.91	0.41
69:3C:504:3PE:H2A2	69:3D:502:3PE:H222	2.02	0.41
69:3C:508:3PE:H262	69:3C:508:3PE:H232	1.86	0.41
69:3C:508:3PE:H2C1	75:3F:201:CDL:H652	2.03	0.41
48:3D:96:PRO:HG3	52:3H:91:ASP:HB3	2.02	0.41
69:3D:503:3PE:H112	49:3E:113:PHE:CE2	2.55	0.41
49:3E:101:LYS:NZ	49:3E:101:LYS:HB2	2.34	0.41
49:3E:254:ALA:C	49:3E:256:LEU:N	2.78	0.41
51:3G:73:ARG:HD2	52:3H:81:GLU:OE1	2.21	0.41
75:3P:513:CDL:H521	75:3P:513:CDL:H112	2.02	0.41
69:3P:518:3PE:H322	69:3P:518:3PE:C27	2.51	0.41
49:3R:227:ASN:O	49:3R:228:ALA:HB2	2.20	0.41
69:3T:103:3PE:H2D2	69:3T:103:3PE:H2A1	1.80	0.41
52:3U:75:ASN:OD1	52:3U:75:ASN:N	2.53	0.41
53:3W:27:VAL:HG12	69:3W:103:3PE:H3F1	2.02	0.41
55:4A:411:LYS:O	55:4A:415:VAL:HG23	2.20	0.41
57:4C:259:TRP:O	68:4N:47:ARG:NH2	2.44	0.41
91:4C:302:PGV:H171	91:4C:302:PGV:H141	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:4D:53:MET:HE3	58:4D:53:MET:HB3	1.88	0.41
69:1B:204:3PE:H361	69:1B:205:3PE:H3B1	2.02	0.41
4:1D:213:GLU:HG2	4:1D:213:GLU:H	1.73	0.41
7:1G:50:GLY:HA2	72:1G:803:FES:S1	2.59	0.41
7:1G:157:THR:HG22	7:1G:161:ARG:HE	1.85	0.41
7:1G:601:ARG:HA	7:1G:611:LEU:HD12	2.02	0.41
13:1M:9:THR:HG21	75:1d:202:CDL:H661	2.03	0.41
75:1N:402:CDL:H782	75:1N:402:CDL:H812	1.87	0.41
16:1P:45:VAL:HG12	16:1P:47:VAL:HG23	2.02	0.41
16:1P:145:TYR:CE1	16:1P:149:LYS:HD2	2.56	0.41
20:1U:3:ALA:HA	20:1U:4:PRO:HD3	1.91	0.41
20:1U:36:PHE:HA	20:1U:40:LEU:HB2	2.02	0.41
21:1V:25:ILE:HG13	21:1V:26:LEU:N	2.34	0.41
23:1X:95:LEU:HB3	23:1X:97:ARG:HG3	2.01	0.41
24:1Y:124:VAL:O	24:1Y:128:GLN:HG3	2.20	0.41
69:1Y:209:3PE:H361	69:1Y:209:3PE:H332	1.73	0.41
75:1Y:217:CDL:H722	69:3S:201:3PE:C22	2.51	0.41
25:1Z:7:LYS:HB2	25:1Z:7:LYS:HE3	1.80	0.41
29:1d:85:LEU:HD23	29:1d:85:LEU:HA	1.92	0.41
75:1d:202:CDL:OB9	69:1f:104:3PE:H282	2.20	0.41
34:1i:15:ARG:HG3	34:1i:19:ARG:HH11	1.85	0.41
75:1q:201:CDL:H532	75:1q:201:CDL:H711	2.03	0.41
44:1s:38:TYR:HD1	44:1s:39:ARG:H	1.68	0.41
45:3A:255:ILE:O	45:3A:321:GLY:HA3	2.20	0.41
45:3A:317:THR:OG1	45:3A:318:GLY:N	2.53	0.41
46:3B:295:LEU:HD23	46:3B:295:LEU:HA	1.90	0.41
47:3C:32:ASN:ND2	47:3C:227:LYS:HE2	2.32	0.41
47:3C:75:TYR:O	47:3C:78:VAL:HG13	2.20	0.41
47:3C:379:TRP:CD2	50:3F:45:ARG:HD3	2.54	0.41
48:3D:153:ALA:O	48:3D:156:VAL:HG22	2.21	0.41
49:3E:155:LYS:HE2	49:3E:155:LYS:H	1.85	0.41
45:3N:445:ARG:NH2	75:3N:502:CDL:O1	2.53	0.41
75:3N:502:CDL:C84	75:3X:103:CDL:H811	2.50	0.41
46:3O:83:PHE:CZ	46:3O:87:ARG:HG3	2.56	0.41
46:3O:435:PHE:HD1	46:3O:438:GLU:OE2	2.03	0.41
75:3P:513:CDL:H542	75:3P:513:CDL:H512	1.71	0.41
69:3P:517:3PE:H3A1	69:3P:518:3PE:H391	2.03	0.41
69:3P:519:3PE:H2H1	69:3P:519:3PE:H2E2	1.77	0.41
48:3Q:37:CYS:SG	86:3Q:501:HEC:C3B	3.08	0.41
49:3R:166:ALA:C	49:3R:167:PHE:CG	2.98	0.41
49:3R:254:ALA:O	49:3R:256:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:3T:19:SER:O	51:3T:23:GLN:HG2	2.20	0.41
69:3W:103:3PE:H322	69:3W:103:3PE:O14	2.21	0.41
54:3X:44:TRP:CD2	69:3X:108:3PE:H372	2.56	0.41
69:3X:101:3PE:H3I1	69:3X:101:3PE:H2C2	2.03	0.41
54:3Y:51:LYS:HE2	54:3Y:51:LYS:HB3	1.78	0.41
55:4A:76:GLY:O	55:4A:80:ASN:HB2	2.20	0.41
91:4G:102:PGV:H132	91:4G:102:PGV:H231	2.02	0.41
63:4I:15:LYS:HE2	63:4I:15:LYS:HB3	1.74	0.41
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.30	0.41
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.20	0.41
3:1C:195:ARG:NH2	9:1I:92:ILE:O	2.53	0.41
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	2.02	0.41
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.53	0.41
5:1E:76:PRO:HA	5:1E:77:PRO:HD3	1.95	0.41
6:1F:16:LYS:HB2	6:1F:16:LYS:HE2	1.80	0.41
6:1F:21:ILE:HG23	6:1F:233:THR:HG21	2.01	0.41
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.33	0.41
7:1G:354:ALA:O	7:1G:357:ASP:HB2	2.21	0.41
12:1L:24:SER:CB	69:1L:710:3PE:H2	2.50	0.41
12:1L:194:ASN:OD1	38:1m:127:SER:HB3	2.20	0.41
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.56	0.41
12:1L:520:TYR:HE2	69:1L:707:3PE:P	2.44	0.41
13:1M:23:ILE:HD13	13:1M:93:LYS:HG3	2.03	0.41
13:1M:78:MET:HE1	13:1M:439:LEU:HD12	2.02	0.41
13:1M:314:ALA:HB2	13:1M:455:LEU:HD23	2.02	0.41
14:1N:256:PRO:HG2	69:1N:401:3PE:C2F	2.47	0.41
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.56	0.41
17:1Q:11:ILE:O	22:1W:16:SER:OG	2.34	0.41
20:1T:37:MET:HE1	20:1T:44:SER:HA	2.02	0.41
23:1X:12:LEU:H	23:1X:12:LEU:HG	1.59	0.41
24:1Y:100:LEU:HD11	69:1Y:205:3PE:O21	2.21	0.41
24:1Y:111:ALA:HB2	69:1Y:213:3PE:H331	2.03	0.41
70:1Y:207:PC1:C27	69:1Y:209:3PE:H372	2.51	0.41
31:1f:14:ILE:C	31:1f:17:PRO:HD2	2.45	0.41
34:1i:46:TRP:CE3	34:1i:50:LEU:HB2	2.54	0.41
35:1j:21:GLN:HG3	35:1j:22:LEU:HD22	2.01	0.41
38:1m:92:PHE:HD1	69:1m:203:3PE:H371	1.75	0.41
39:1n:149:ARG:HA	39:1n:149:ARG:HD2	1.88	0.41
40:1o:85:ASP:OD1	40:1o:85:ASP:N	2.53	0.41
45:3A:3:THR:O	45:3A:4:TYR:HB3	2.20	0.41
45:3A:170:PRO:HB2	45:3A:172:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:3B:44:ALA:HA	46:3B:112:LEU:HA	2.02	0.41
46:3B:202:ALA:HB3	46:3B:229:GLY:O	2.21	0.41
46:3B:290:ASN:O	46:3B:297:GLN:NE2	2.53	0.41
47:3C:45:ILE:HA	85:3C:501:HEM:CMC	2.50	0.41
47:3C:100:ARG:NH2	85:3C:502:HEM:HBD1	2.36	0.41
47:3C:331:ASP:OD1	47:3C:357:LEU:HD23	2.20	0.41
47:3C:360:LEU:HD21	69:3C:507:3PE:H3F1	2.03	0.41
69:3C:511:3PE:H241	69:3C:511:3PE:H272	1.81	0.41
48:3D:245:GLN:CG	52:3H:84:PHE:HZ	2.29	0.41
75:3D:504:CDL:H321	51:3G:32:PHE:CD1	2.56	0.41
49:3E:159:ILE:HG12	49:3E:165:MET:HB2	2.02	0.41
49:3E:184:ILE:CG2	49:3E:185:ASP:N	2.84	0.41
49:3E:219:HIS:ND1	49:3E:219:HIS:O	2.53	0.41
50:3F:24:TRP:CD1	50:3F:26:GLU:HB2	2.55	0.41
50:3F:52:ASP:O	50:3F:56:LYS:HG3	2.21	0.41
45:3N:52:ASN:O	45:3N:53:ASN:C	2.63	0.41
45:3N:108:LYS:HE3	45:3N:112:LEU:CD1	2.50	0.41
46:3O:276:GLN:HG2	46:3O:281:ALA:HB2	2.02	0.41
47:3P:240:LEU:HD13	48:3Q:208:MET:HG3	2.03	0.41
75:3P:513:CDL:H231	69:3P:520:3PE:C2F	2.44	0.41
49:3R:207:LYS:O	49:3R:209:GLU:N	2.53	0.41
53:3W:23:LEU:CD2	54:3X:23:MET:HE3	2.51	0.41
54:3Y:33:VAL:CB	69:3Y:105:3PE:H2H1	2.51	0.41
56:4B:172:THR:OG1	62:4H:23:GLN:NE2	2.54	0.41
57:4C:108:PRO:O	62:4H:27:ARG:NH1	2.51	0.41
59:4E:43:PRO:HB2	59:4E:48:ILE:HD11	2.01	0.41
91:4N:101:PGV:H41	91:4N:101:PGV:H72	1.86	0.41
2:1B:62:MET:O	2:1B:68:ASP:N	2.53	0.41
70:1B:202:PC1:H372	70:1B:202:PC1:H342	1.85	0.41
5:1E:168:ASP:HA	5:1E:171:GLU:HG2	2.03	0.41
7:1G:526:GLY:N	7:1G:546:GLN:O	2.53	0.41
8:1H:30:TYR:HE1	26:1a:1:MET:HB2	1.84	0.41
8:1H:98:MET:HB3	70:1H:403:PC1:O12	2.21	0.41
8:1H:100:LEU:HD23	8:1H:160:TYR:HB2	2.03	0.41
8:1H:100:LEU:HD22	8:1H:103:LEU:HD12	2.02	0.41
8:1H:149:ILE:HG12	8:1H:181:LEU:HD22	2.02	0.41
70:1H:402:PC1:H372	9:1I:25:LEU:HB3	2.02	0.41
9:1I:44:GLU:CD	76:1I:203:AYA:C	2.94	0.41
12:1L:138:PHE:HD2	69:1L:702:3PE:H3G2	1.85	0.41
13:1M:53:SER:C	13:1M:55:THR:N	2.77	0.41
16:1P:20:VAL:HG13	16:1P:44:GLN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:274:PRO:HG2	16:1P:275:PHE:CZ	2.55	0.41
17:1Q:67:ASN:HB3	17:1Q:72:TRP:H	1.86	0.41
24:1Y:79:VAL:CG1	69:1Y:214:3PE:H232	2.47	0.41
69:1Y:209:3PE:H392	69:1Y:213:3PE:H261	2.01	0.41
69:1Y:215:3PE:H2E1	70:3T:102:PC1:C3A	2.47	0.41
32:1g:67:SER:O	33:1h:32:THR:OG1	2.33	0.41
37:1l:91:THR:HG22	38:1m:10:LEU:HA	2.02	0.41
41:1p:14:ARG:HG2	41:1p:14:ARG:NH1	2.35	0.41
41:1p:92:ARG:O	41:1p:96:LYS:HE2	2.21	0.41
45:3A:184:GLU:O	45:3A:188:GLN:HG2	2.21	0.41
46:3B:70:ARG:HG2	49:3I:68:VAL:CG2	2.50	0.41
47:3C:284:ILE:HA	47:3C:285:PRO:HD3	1.95	0.41
47:3C:359:PHE:HB2	69:3C:512:3PE:H2F1	2.03	0.41
69:3J:105:3PE:H2E1	69:3Y:102:3PE:H382	2.02	0.41
47:3P:222:PRO:HG2	47:3P:223:TYR:CD2	2.55	0.41
75:3P:513:CDL:H351	75:3P:513:CDL:H382	1.81	0.41
49:3R:170:ARG:C	49:3R:172:LYS:N	2.73	0.41
49:3R:234:TYR:HD2	49:3R:243:TYR:HB2	1.83	0.41
69:3W:103:3PE:O22	69:3W:103:3PE:H11	2.19	0.41
54:3Y:4:ARG:HH21	69:3Y:107:3PE:P	2.34	0.41
55:4A:177:SER:HB3	55:4A:180:GLN:HG3	2.01	0.41
55:4A:273:MET:HE1	55:4A:323:TRP:CD1	2.55	0.41
55:4A:430:PHE:HB3	56:4B:7:LEU:HA	2.02	0.41
75:4B:302:CDL:H821	75:4B:302:CDL:H792	1.77	0.41
57:4C:132:LEU:HD11	61:4G:32:THR:HA	2.03	0.41
59:4E:81:ILE:HG23	63:4I:9:MET:SD	2.60	0.41
62:4H:48:GLY:O	62:4H:50:VAL:HG23	2.21	0.41
4:1D:66:MET:HG2	4:1D:76:CYS:HA	2.03	0.41
4:1D:170:MET:HE2	4:1D:225:LEU:HD22	2.02	0.41
4:1D:309:ARG:HG3	25:1Z:21:TYR:CE2	2.55	0.41
8:1H:91:MET:HE3	8:1H:91:MET:HB2	1.90	0.41
10:1J:7:PHE:CE1	11:1K:3:LEU:HD22	2.50	0.41
11:1K:38:LEU:O	11:1K:42:ILE:HD12	2.21	0.41
12:1L:297:ASP:O	12:1L:301:ILE:HG22	2.21	0.41
69:1L:712:3PE:H2A2	69:1L:712:3PE:H2D2	1.79	0.41
13:1M:105:PHE:O	13:1M:109:THR:OG1	2.29	0.41
15:1O:35:LYS:O	15:1O:39:ALA:N	2.45	0.41
15:1O:80:GLU:N	15:1O:80:GLU:CD	2.79	0.41
16:1P:301:GLU:H	16:1P:301:GLU:CD	2.29	0.41
20:1T:54:MET:HB3	20:1T:58:PHE:CD2	2.55	0.41
20:1U:6:LEU:HD23	20:1U:6:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:57:GLU:OE2	35:1j:12:ARG:NH2	2.31	0.41
24:1Y:109:ILE:HG23	70:1Y:206:PC1:H332	2.02	0.41
69:1f:101:3PE:H351	69:1f:101:3PE:H391	2.03	0.41
69:1m:201:3PE:H2A1	69:1m:201:3PE:H2D1	1.87	0.41
39:1n:64:ARG:NE	39:1n:64:ARG:HA	2.36	0.41
45:3A:326:CYS:HB2	45:3A:330:SER:OG	2.21	0.41
45:3A:339:GLN:O	45:3A:343:MET:HG2	2.20	0.41
47:3C:236:MET:HE2	69:3E:303:3PE:H281	2.02	0.41
69:3D:502:3PE:H391	69:3D:502:3PE:H261	2.02	0.41
49:3E:154:ILE:HD12	49:3E:154:ILE:C	2.46	0.41
50:3F:113:ARG:O	50:3F:117:GLU:HG3	2.20	0.41
69:3G:103:3PE:H251	69:3G:108:3PE:C24	2.38	0.41
69:3G:110:3PE:O13	69:3G:111:3PE:H11	2.19	0.41
69:3J:104:3PE:H3E1	69:3J:104:3PE:H3H2	1.81	0.41
45:3N:241:ILE:CD1	49:3R:83:ILE:HD11	2.50	0.41
46:3O:36:ALA:HB3	46:3O:207:ILE:HD12	2.03	0.41
47:3P:221:HIS:HA	47:3P:225:THR:HG23	2.01	0.41
47:3P:229:ILE:HG21	70:3R:303:PC1:H351	2.03	0.41
47:3P:234:PHE:CD2	75:3T:101:CDL:H532	2.56	0.41
69:3P:503:3PE:H282	69:3P:518:3PE:C33	2.51	0.41
49:3R:80:HIS:O	49:3R:83:ILE:HG23	2.21	0.41
69:3X:101:3PE:H231	69:3X:101:3PE:H382	2.03	0.41
54:3Y:41:ILE:HA	69:3Y:105:3PE:H371	2.02	0.41
55:4A:11:ASN:O	55:4A:15:ILE:HG13	2.21	0.41
56:4B:179:LEU:HD21	62:4H:63:PHE:O	2.20	0.41
57:4C:158:HIS:HE2	60:4F:1:ALA:HA	1.86	0.41
58:4D:54:ASP:OD1	58:4D:54:ASP:N	2.53	0.41
60:4F:10:GLU:OE1	60:4F:10:GLU:C	2.64	0.41
69:1A:201:3PE:H321	69:1b:101:3PE:H2	2.02	0.41
69:1A:203:3PE:H2B2	69:1A:203:3PE:H381	2.03	0.41
2:1B:45:LEU:HD23	2:1B:45:LEU:HA	1.85	0.41
3:1C:40:VAL:HG22	43:1r:69:MET:HB3	2.02	0.41
4:1D:4:TRP:CE2	13:1M:140:THR:HB	2.56	0.41
4:1D:69:SER:HB3	4:1D:74:ARG:HD3	2.02	0.41
4:1D:108:TYR:CZ	4:1D:424:VAL:HG13	2.56	0.41
6:1F:22:PHE:HB2	6:1F:25:LEU:HB2	2.03	0.41
6:1F:205:LEU:H	6:1F:205:LEU:HD12	1.85	0.41
7:1G:621:SER:O	7:1G:625:GLU:HG3	2.21	0.41
9:1I:50:TYR:CD1	9:1I:51:PRO:HA	2.56	0.41
9:1I:155:LEU:HD23	9:1I:155:LEU:HA	1.88	0.41
10:1J:66:VAL:O	10:1J:70:TYR:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:68:PHE:CE2	11:1K:30:LEU:HD13	2.56	0.41
10:1J:106:TYR:HA	10:1J:110:GLU:OE2	2.21	0.41
11:1K:21:MET:HE2	11:1K:21:MET:HB3	1.89	0.41
12:1L:12:LEU:HD22	12:1L:129:MET:HB3	2.02	0.41
12:1L:67:HIS:HE2	12:1L:70:THR:HB	1.86	0.41
12:1L:205:ASN:O	12:1L:207:GLU:N	2.54	0.41
13:1M:14:MET:HE1	13:1M:27:ALA:HA	2.03	0.41
13:1M:74:PRO:HA	13:1M:77:LEU:HD12	2.02	0.41
70:1M:501:PC1:H153	75:1i:201:CDL:OA3	2.21	0.41
14:1N:6:TYR:O	14:1N:10:ILE:HG12	2.20	0.41
14:1N:40:MET:HE3	14:1N:134:GLN:CD	2.46	0.41
14:1N:277:ILE:HG12	82:1Y:203:PGT:C16	2.51	0.41
15:1O:260:ARG:HE	15:1O:260:ARG:HB2	1.76	0.41
16:1P:19:ILE:HD13	16:1P:218:ILE:HG21	2.03	0.41
16:1P:99:TRP:CE2	16:1P:277:PRO:HD2	2.56	0.41
16:1P:268:ARG:HA	16:1P:268:ARG:HD2	1.92	0.41
16:1P:294:LEU:HB3	16:1P:296:HIS:CE1	2.56	0.41
23:1X:144:ARG:HD2	30:1e:57:ILE:HD11	2.02	0.41
24:1Y:31:THR:HG21	69:1Y:208:3PE:C2C	2.48	0.41
69:1Y:201:3PE:H3A2	69:1Y:201:3PE:H371	1.85	0.41
75:1Y:217:CDL:H1O1	69:3S:201:3PE:P	2.43	0.41
75:1Y:217:CDL:H742	69:3S:201:3PE:H242	2.03	0.41
25:1Z:6:VAL:HG11	43:1r:41:PRO:HB3	2.03	0.41
27:1b:58:ASP:OD1	27:1b:58:ASP:O	2.39	0.41
27:1b:81:LYS:HB2	27:1b:81:LYS:HE3	1.78	0.41
29:1d:60:ARG:CG	75:1d:205:CDL:HB32	2.47	0.41
31:1f:22:PHE:HZ	69:1f:104:3PE:H242	1.84	0.41
31:1f:28:ARG:HB3	31:1f:29:ARG:HH12	1.86	0.41
75:1g:201:CDL:H632	75:1g:201:CDL:H661	1.80	0.41
75:1g:201:CDL:OA7	69:1g:203:3PE:H222	2.21	0.41
33:1h:23:LYS:HB3	33:1h:23:LYS:HE3	1.74	0.41
70:1h:203:PC1:H391	69:1h:204:3PE:C2E	2.51	0.41
45:3A:79:VAL:HG22	45:3A:112:LEU:HD13	2.03	0.41
45:3A:140:GLU:O	45:3A:143:SER:OG	2.37	0.41
45:3A:178:SER:O	45:3A:182:LEU:HG	2.21	0.41
46:3B:76:THR:HG22	46:3B:131:GLU:OE2	2.21	0.41
47:3C:158:THR:O	47:3C:162:GLU:HG3	2.21	0.41
69:3C:509:3PE:H3H1	75:3N:502:CDL:C87	2.45	0.41
69:3C:510:3PE:H252	69:3C:510:3PE:H281	1.81	0.41
69:3C:517:3PE:H242	69:3C:517:3PE:C28	2.45	0.41
48:3D:226:PRO:HD2	48:3D:229:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:3D:503:3PE:H271	69:3G:102:3PE:H382	2.02	0.41
75:3D:504:CDL:H321	51:3G:32:PHE:CE1	2.56	0.41
49:3E:179:ARG:HG3	49:3E:211:VAL:N	2.31	0.41
49:3E:199:GLN:NE2	49:3E:203:GLU:HG2	2.35	0.41
49:3E:216:VAL:HG21	47:3P:262:LEU:HD22	2.02	0.41
49:3E:234:TYR:C	49:3E:243:TYR:HB2	2.46	0.41
49:3E:257:ASN:O	49:3E:258:LEU:C	2.64	0.41
52:3H:45:VAL:HG12	52:3H:94:VAL:HG22	2.03	0.41
52:3H:65:CYS:O	52:3H:69:VAL:HG23	2.20	0.41
49:3I:42:VAL:O	49:3I:43:LEU:HB2	2.19	0.41
45:3N:19:LEU:HD22	45:3N:213:GLN:HG2	2.03	0.41
45:3N:240:GLU:OE2	45:3N:242:ARG:NH2	2.54	0.41
45:3N:416:TYR:CE1	45:3N:442:PHE:HA	2.55	0.41
69:3N:503:3PE:H371	69:3N:503:3PE:H262	2.02	0.41
46:3O:29:LEU:HD12	46:3O:33:LEU:HD12	2.02	0.41
46:3O:120:MET:O	46:3O:124:LEU:HG	2.20	0.41
46:3O:181:TYR:CE2	46:3O:182:ARG:HG2	2.56	0.41
46:3O:307:PHE:H	49:3V:52:ARG:HG3	1.84	0.41
47:3P:116:GLY:HA3	85:3P:502:HEM:C3C	2.56	0.41
47:3P:249:LEU:HA	69:3P:520:3PE:O12	2.21	0.41
47:3P:306:MET:CE	69:3P:514:3PE:H241	2.43	0.41
69:3P:510:3PE:C31	69:3P:510:3PE:H352	2.51	0.41
69:3P:514:3PE:H382	69:3P:514:3PE:H3B2	1.77	0.41
69:3P:517:3PE:H3G1	69:3P:517:3PE:H3D2	1.80	0.41
48:3Q:16:GLY:O	48:3Q:202:LYS:NZ	2.48	0.41
49:3R:196:ARG:NH2	49:3R:254:ALA:O	2.54	0.41
49:3R:241:SER:CB	49:3R:249:ILE:HG23	2.50	0.41
69:3R:304:3PE:H2E1	69:3R:304:3PE:H2B2	1.92	0.41
52:3U:43:ARG:NH1	52:3U:52:GLU:OE2	2.54	0.41
69:3W:101:3PE:H251	69:3W:102:3PE:C3	2.51	0.41
69:3W:101:3PE:H32	69:3W:101:3PE:O13	2.21	0.41
55:4A:230:LEU:O	55:4A:233:HIS:HB2	2.20	0.41
55:4A:328:HIS:NE2	63:4I:17:LEU:HD22	2.36	0.41
55:4A:423:MET:CE	91:4K:101:PGV:C34	2.98	0.41
55:4A:443:TYR:O	56:4B:134:ARG:NH2	2.54	0.41
56:4B:106:TRP:CE2	56:4B:207:MET:HE2	2.56	0.41
57:4C:86:PHE:HE1	91:4C:301:PGV:H292	1.85	0.41
75:4C:306:CDL:H372	75:4C:306:CDL:H401	1.83	0.41
59:4E:10:GLU:HG3	59:4E:11:PHE:N	2.36	0.41
61:4G:54:ARG:HB3	61:4G:79:PRO:HG3	2.03	0.41
61:4G:55:ILE:HG22	61:4G:57:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:4M:11:SER:HB3	67:4M:14:GLU:HG3	2.03	0.41
68:4N:41:PRO:HA	68:4N:53:PRO:O	2.21	0.41
1:1A:24:LEU:N	1:1A:25:PRO:CD	2.84	0.41
2:1B:48:MET:HE2	2:1B:50:PHE:HD1	1.85	0.41
2:1B:154:GLU:OE2	9:1I:54:LYS:HB3	2.21	0.41
3:1C:175:ARG:NH1	3:1C:177:ASP:OD2	2.44	0.41
3:1C:177:ASP:HB3	3:1C:180:VAL:HG22	2.02	0.41
4:1D:260:LEU:HD22	4:1D:265:ILE:HD13	2.03	0.41
6:1F:190:THR:CB	6:1F:204:ARG:H	2.34	0.41
6:1F:255:LEU:HD23	6:1F:255:LEU:HA	1.98	0.41
6:1F:366:ARG:CZ	7:1G:155:GLN:HB2	2.51	0.41
6:1F:418:LEU:HD22	6:1F:422:PHE:HB2	2.03	0.41
7:1G:284:ILE:HG23	7:1G:294:THR:HG21	2.03	0.41
8:1H:35:LYS:HD2	9:1I:47:THR:HB	2.03	0.41
8:1H:181:LEU:HG	8:1H:300:LEU:HD13	2.03	0.41
8:1H:277:TYR:OH	9:1I:30:LEU:O	2.37	0.41
9:1I:70:TYR:CE2	9:1I:76:ARG:HG2	2.55	0.41
12:1L:76:LEU:HB3	69:1L:702:3PE:C3I	2.51	0.41
12:1L:562:LEU:HB2	12:1L:563:PRO:HD3	2.01	0.41
13:1M:256:TYR:CD1	13:1M:256:TYR:C	2.98	0.41
14:1N:296:LEU:HA	14:1N:296:LEU:HD23	1.84	0.41
16:1P:139:ILE:HG23	16:1P:140:LYS:HG2	2.02	0.41
16:1P:157:ARG:HA	16:1P:157:ARG:HD3	1.88	0.41
16:1P:172:PHE:HB2	16:1P:179:LEU:HD21	2.03	0.41
20:1T:58:PHE:CD1	20:1T:80:ILE:HG21	2.55	0.41
20:1T:64:ASP:OD1	22:1W:30:ARG:NH2	2.51	0.41
20:1U:19:LEU:C	20:1U:21:LEU:H	2.28	0.41
23:1X:40:LYS:HD2	27:1b:55:PRO:HG3	2.03	0.41
24:1Y:120:THR:HG23	69:1Y:211:3PE:H2C2	2.03	0.41
69:1Y:209:3PE:C38	75:3P:513:CDL:H852	2.50	0.41
69:1d:201:3PE:H321	69:1d:201:3PE:H282	2.03	0.41
75:1d:205:CDL:HB31	75:1d:205:CDL:CB2	2.51	0.41
31:1f:28:ARG:NH2	69:1f:103:3PE:O11	2.53	0.41
33:1h:41:THR:O	33:1h:45:VAL:HG13	2.21	0.41
34:1i:83:TYR:HE2	75:1i:201:CDL:H511	1.76	0.41
40:1o:73:PHE:CG	40:1o:74:PRO:HA	2.56	0.41
47:3C:245:PHE:CD1	48:3D:105:LEU:HG	2.56	0.41
69:3C:513:3PE:H372	69:3C:517:3PE:H372	2.03	0.41
49:3E:222:CYS:O	49:3E:223:VAL:C	2.63	0.41
69:3G:104:3PE:H221	69:3G:104:3PE:H2	1.79	0.41
45:3N:272:VAL:HG21	45:3N:402:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3N:445:ARG:CG	75:3N:502:CDL:OB3	2.54	0.41
69:3N:501:3PE:H242	75:3X:103:CDL:H582	2.03	0.41
46:3O:78:LYS:HG3	46:3O:129:ALA:HB1	2.03	0.41
47:3P:360:LEU:O	47:3P:365:LEU:HG	2.20	0.41
69:3P:516:3PE:H281	69:3P:516:3PE:H252	1.93	0.41
49:3R:254:ALA:C	49:3R:256:LEU:N	2.79	0.41
70:3T:102:PC1:H281	70:3T:102:PC1:H252	1.93	0.41
52:3U:27:ILE:HG13	52:3U:30:CYS:H	1.86	0.41
69:3Y:101:3PE:H3D1	69:3Y:105:3PE:H3G2	2.02	0.41
69:3Y:102:3PE:H3B2	69:3Y:105:3PE:H3E2	2.01	0.41
55:4A:302:ARG:NH2	56:4B:88:ASP:OD1	2.54	0.41
55:4A:418:PHE:HE2	91:4A:608:PGV:C10	2.33	0.41
55:4A:470:PHE:CG	67:4M:19:LEU:HD13	2.56	0.41
55:4A:477:ALA:HB1	66:4L:18:LYS:NZ	2.35	0.41
55:4A:495:LEU:HD23	55:4A:495:LEU:HA	1.87	0.41
91:4C:302:PGV:H281	91:4C:302:PGV:H242	2.02	0.41
61:4G:48:ILE:O	61:4G:50:TYR:N	2.50	0.41
1:1A:5:LEU:HD21	8:1H:3:MET:CE	2.51	0.40
1:1A:73:LEU:HD23	8:1H:151:LEU:HD12	2.03	0.40
2:1B:68:ASP:OD2	8:1H:34:ARG:HB3	2.21	0.40
2:1B:77:ARG:NH1	2:1B:78:ALA:HB3	2.36	0.40
4:1D:52:GLY:N	4:1D:53:PRO:CD	2.84	0.40
4:1D:232:ASN:O	4:1D:236:ARG:HG3	2.21	0.40
7:1G:317:ALA:HB1	7:1G:331:LEU:HD21	2.02	0.40
8:1H:124:ASN:HB3	8:1H:125:SER:H	1.65	0.40
12:1L:146:GLY:HA3	75:1L:704:CDL:H762	2.02	0.40
12:1L:281:GLY:HA3	12:1L:314:MET:HB3	2.03	0.40
12:1L:296:ASN:ND2	12:1L:425:ARG:HH12	2.20	0.40
69:1L:708:3PE:H331	69:1L:708:3PE:H362	1.93	0.40
13:1M:220:HIS:NE2	13:1M:231:LEU:HB3	2.36	0.40
14:1N:222:SER:HA	14:1N:237:MET:CE	2.51	0.40
69:1N:401:3PE:H381	69:1N:401:3PE:H3B1	1.93	0.40
15:1O:31:ILE:HD12	15:1O:31:ILE:N	2.34	0.40
17:1Q:124:TRP:HD1	17:1Q:125:ASN:OD1	2.04	0.40
17:1Q:124:TRP:O	44:1s:68:SER:OG	2.29	0.40
23:1X:36:ASP:OD2	27:1b:69:PRO:HD3	2.21	0.40
24:1Y:75:ILE:CG2	69:1Y:214:3PE:C28	2.89	0.40
69:1Y:201:3PE:H3C1	69:1Y:201:3PE:H391	1.71	0.40
69:1Y:209:3PE:H262	69:1Y:209:3PE:H231	1.90	0.40
69:1Y:209:3PE:H252	69:1Y:209:3PE:H281	1.86	0.40
69:1Y:209:3PE:H352	75:3P:513:CDL:H842	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
69:1Y:215:3PE:H3B2	69:3P:517:3PE:H2I1	2.03	0.40
26:1a:55:SER:HB2	26:1a:62:VAL:HG13	2.02	0.40
31:1f:10:HIS:CE1	69:1f:102:3PE:C21	3.04	0.40
75:1g:201:CDL:CA3	69:1g:203:3PE:H122	2.52	0.40
34:1i:100:LYS:HG3	40:1o:49:GLN:HE21	1.86	0.40
34:1i:105:PRO:HG2	34:1i:119:MET:HE1	2.03	0.40
37:1l:50:LEU:HD11	37:1l:76:PRO:HB2	2.03	0.40
38:1m:47:LEU:HB3	39:1n:165:LEU:HD13	2.03	0.40
39:1n:10:THR:O	39:1n:14:LYS:HG3	2.21	0.40
45:3A:61:HIS:HB3	45:3A:130:GLU:CG	2.50	0.40
45:3A:363:ASN:ND2	46:3B:93:GLY:HA3	2.36	0.40
75:3A:501:CDL:H641	69:3A:502:3PE:C2H	2.51	0.40
46:3B:358:GLN:HE21	46:3B:362:ASN:HD21	1.69	0.40
47:3C:222:PRO:HG2	47:3C:223:TYR:CD2	2.56	0.40
69:3C:512:3PE:H261	69:3C:512:3PE:H341	2.02	0.40
48:3D:326:TYR:HE1	51:3G:14:HIS:HB2	1.87	0.40
49:3E:236:CYS:SG	72:3E:301:FES:S2	3.19	0.40
75:3F:201:CDL:H791	75:3F:201:CDL:H582	2.03	0.40
45:3N:37:VAL:HG21	45:3N:110:VAL:HG22	2.03	0.40
45:3N:67:THR:HG22	45:3N:119:ASN:C	2.47	0.40
75:3N:502:CDL:H861	75:3X:103:CDL:C81	2.42	0.40
46:3O:45:SER:CB	46:3O:116:ILE:HG13	2.51	0.40
75:3P:513:CDL:H601	75:3P:513:CDL:H632	1.91	0.40
48:3Q:150:ASN:HA	48:3Q:151:PRO:HD2	1.91	0.40
48:3Q:195:GLU:OE1	48:3Q:201:ARG:NE	2.52	0.40
48:3Q:214:LEU:C	48:3Q:217:PRO:HD2	2.47	0.40
49:3R:133:VAL:HG11	69:3R:304:3PE:H3B2	2.03	0.40
50:3S:19:TRP:CE2	69:3S:201:3PE:H322	2.56	0.40
75:3T:101:CDL:C34	75:3T:101:CDL:CA7	2.99	0.40
53:3W:34:ARG:HG2	54:3X:47:TYR:CZ	2.56	0.40
69:3W:103:3PE:H3C1	69:3W:103:3PE:H392	1.78	0.40
70:3X:104:PC1:H3C2	70:3X:104:PC1:H391	1.67	0.40
55:4A:409:TRP:HA	55:4A:412:ILE:HD12	2.03	0.40
55:4A:512:ASN:HD21	60:4F:38:ALA:HA	1.85	0.40
91:4A:606:PGV:H61	91:4A:606:PGV:H32	1.93	0.40
91:4A:609:PGV:H311	91:4A:609:PGV:H282	1.85	0.40
56:4B:110:TYR:CD1	56:4B:116:LEU:HD22	2.57	0.40
58:4D:131:ILE:HG12	63:4I:50:PHE:CD2	2.56	0.40
59:4E:71:VAL:HG11	59:4E:85:VAL:HG11	2.03	0.40
62:4H:25:GLN:HG2	62:4H:63:PHE:HE2	1.86	0.40
67:4M:37:LEU:HD23	67:4M:37:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:54:LYS:HE2	1:1A:54:LYS:HB2	1.51	0.40
1:1A:95:LEU:HD13	8:1H:302:MET:HG3	2.03	0.40
3:1C:199:LEU:HD12	4:1D:385:ARG:HH11	1.86	0.40
4:1D:335:ARG:NH2	9:1I:129:ASP:OD1	2.51	0.40
5:1E:120:ILE:HG22	5:1E:139:LEU:HD22	2.03	0.40
5:1E:187:ARG:HD3	5:1E:187:ARG:HA	1.86	0.40
6:1F:111:ILE:HD13	6:1F:138:ILE:HD13	2.04	0.40
6:1F:349:ARG:HA	6:1F:349:ARG:HD2	1.83	0.40
8:1H:10:ILE:HG23	8:1H:83:LEU:HD22	2.03	0.40
70:1H:402:PC1:C3E	27:1b:24:ILE:HD11	2.51	0.40
12:1L:568:PHE:CZ	12:1L:572:LYS:HD3	2.55	0.40
15:1O:137:ALA:O	15:1O:138:MET:C	2.63	0.40
16:1P:325:ARG:HG3	16:1P:326:TRP:CE2	2.56	0.40
26:1a:41:PHE:O	26:1a:44:GLN:N	2.54	0.40
29:1d:120:ARG:O	38:1m:108:ARG:NH2	2.36	0.40
75:1g:201:CDL:H771	33:1h:35:PRO:HG3	2.03	0.40
35:1j:43:ASP:C	35:1j:43:ASP:OD1	2.64	0.40
39:1n:9:LEU:HB3	39:1n:14:LYS:HE3	2.03	0.40
39:1n:100:GLU:HB2	39:1n:121:ARG:HH12	1.87	0.40
45:3A:27:SER:OG	45:3A:205:HIS:HB2	2.21	0.40
46:3B:78:LYS:HA	46:3B:131:GLU:OE1	2.22	0.40
46:3B:182:ARG:NH1	46:3B:190:GLN:HE22	2.19	0.40
47:3C:141:TRP:HB3	47:3C:268:ILE:CD1	2.47	0.40
48:3D:108:SER:OG	53:3J:51:LYS:HE3	2.21	0.40
49:3E:214:ILE:HD13	49:3E:214:ILE:HA	1.95	0.40
49:3E:268:ASP:C	49:3E:270:LEU:N	2.77	0.40
53:3J:39:GLY:HA3	69:3J:104:3PE:H3A1	2.03	0.40
45:3N:112:LEU:HD12	45:3N:112:LEU:HA	1.88	0.40
45:3N:266:ASP:C	45:3N:269:PRO:HD2	2.47	0.40
46:3O:167:ALA:C	46:3O:240:ARG:HG2	2.47	0.40
46:3O:354:ASN:ND2	46:3O:358:GLN:HG2	2.36	0.40
47:3P:62:ALA:O	47:3P:66:VAL:HG23	2.20	0.40
47:3P:117:VAL:N	85:3P:502:HEM:HBC2	2.36	0.40
69:3P:504:3PE:H252	69:3P:504:3PE:H221	1.84	0.40
69:3P:504:3PE:H261	69:3Y:103:3PE:C23	2.51	0.40
69:3Q:502:3PE:H251	69:3Q:502:3PE:H371	2.03	0.40
69:3Q:503:3PE:H2G2	69:3W:101:3PE:H2I3	2.02	0.40
69:3Q:503:3PE:H391	69:3W:101:3PE:H352	2.03	0.40
49:3R:163:LYS:HZ3	49:3R:163:LYS:HB2	1.85	0.40
49:3R:241:SER:HA	49:3R:249:ILE:HG23	2.04	0.40
69:3T:103:3PE:H2B2	69:3T:103:3PE:C24	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:94:PHE:HB3	91:4C:301:PGV:O13	2.21	0.40
55:4A:510:TYR:HB3	60:4F:58:VAL:HG22	2.03	0.40
56:4B:28:LEU:HD12	56:4B:28:LEU:HA	1.86	0.40
75:4B:302:CDL:H311	75:4B:302:CDL:H342	1.62	0.40
57:4C:84:ILE:O	57:4C:88:ILE:HG13	2.21	0.40
75:4C:307:CDL:H601	75:4C:307:CDL:H631	1.85	0.40
3:1C:43:SER:HA	43:1r:65:PRO:HB3	2.03	0.40
4:1D:152:MET:HE2	4:1D:152:MET:HB2	1.82	0.40
5:1E:127:LYS:O	5:1E:130:GLU:HG2	2.22	0.40
6:1F:342:ASP:HB3	6:1F:345:LYS:HB3	2.03	0.40
7:1G:288:LYS:HD2	7:1G:290:LEU:HD13	2.03	0.40
7:1G:371:VAL:HG21	7:1G:395:ILE:HA	2.03	0.40
8:1H:70:MET:HA	8:1H:73:ILE:HB	2.03	0.40
9:1I:22:ALA:HB2	25:1Z:36:PHE:CE2	2.55	0.40
9:1I:47:THR:O	42:1q:58:ARG:HD2	2.21	0.40
70:1J:202:PC1:H142	70:1J:202:PC1:H112	1.72	0.40
11:1K:4:VAL:O	11:1K:8:ILE:HG12	2.22	0.40
11:1K:16:LEU:HA	11:1K:36:MET:SD	2.62	0.40
12:1L:291:CYS:O	12:1L:295:GLN:HG2	2.21	0.40
12:1L:500:LEU:HD13	64:4J:33:ARG:HD3	1.90	0.40
75:1L:704:CDL:H802	13:1M:371:PRO:HD3	2.02	0.40
14:1N:3:PRO:O	14:1N:7:THR:HG23	2.22	0.40
14:1N:277:ILE:CG1	82:1Y:203:PGT:C16	2.98	0.40
16:1P:59:LEU:HA	16:1P:62:MET:SD	2.62	0.40
21:1V:29:LYS:O	21:1V:33:VAL:HG23	2.21	0.40
22:1W:17:VAL:HG21	22:1W:77:ARG:CZ	2.52	0.40
24:1Y:124:VAL:CG2	69:1Y:211:3PE:H282	2.39	0.40
82:1Y:203:PGT:H391	82:1Y:203:PGT:H421	1.92	0.40
69:1Y:205:3PE:O12	69:1Y:208:3PE:H12	2.21	0.40
70:1Y:207:PC1:H391	70:1Y:207:PC1:H362	1.84	0.40
75:1Y:217:CDL:C21	69:3S:201:3PE:H3C2	2.44	0.40
26:1a:6:LEU:N	26:1a:7:PRO:CD	2.84	0.40
27:1b:34:LEU:H	27:1b:34:LEU:HG	1.62	0.40
28:1c:1:LYS:HE3	28:1c:1:LYS:HB2	1.95	0.40
29:1d:53:VAL:CG2	69:1d:201:3PE:H221	2.51	0.40
29:1d:86:ARG:HD3	83:1h:201:AME:HE1	2.03	0.40
69:1e:201:3PE:H2A1	69:1e:201:3PE:H2D1	1.88	0.40
69:1l:204:3PE:H352	69:1l:204:3PE:O31	2.22	0.40
39:1n:41:CYS:O	39:1n:45:ALA:N	2.45	0.40
42:1q:22:GLY:O	42:1q:26:VAL:HG22	2.21	0.40
75:1q:202:CDL:H602	75:1q:202:CDL:C17	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3A:68:LYS:HB3	45:3A:68:LYS:HE3	1.53	0.40
46:3B:201:SER:C	46:3B:203:ARG:H	2.30	0.40
46:3B:272:PHE:HZ	46:3B:416:LYS:HD3	1.86	0.40
47:3C:161:VAL:HG13	47:3C:162:GLU:N	2.36	0.40
69:3C:511:3PE:H332	69:3C:511:3PE:H362	1.94	0.40
69:3C:511:3PE:H251	69:3C:511:3PE:C21	2.50	0.40
69:3G:102:3PE:H11	69:3G:102:3PE:O22	2.20	0.40
52:3H:43:THR:O	52:3H:47:GLU:HG2	2.22	0.40
69:3J:103:3PE:O31	69:3J:103:3PE:C21	2.70	0.40
69:3N:501:3PE:C2C	75:3N:502:CDL:H581	2.36	0.40
75:3N:502:CDL:H221	75:3N:502:CDL:H251	1.92	0.40
47:3P:21:LEU:HA	47:3P:22:PRO:HD3	1.91	0.40
69:3P:506:3PE:H221	69:3P:506:3PE:H2	1.94	0.40
75:3P:513:CDL:H531	75:3P:513:CDL:H562	1.91	0.40
48:3Q:3:LEU:HD11	52:3U:56:GLU:HA	2.03	0.40
48:3Q:27:ARG:HG2	48:3Q:31:GLN:HE21	1.85	0.40
49:3R:153:GLU:HG3	49:3R:169:TRP:CE3	2.56	0.40
49:3R:235:TYR:HE1	49:3R:237:PRO:HA	1.86	0.40
53:3W:30:LEU:HD12	54:3X:34:TRP:HD1	1.86	0.40
53:3W:52:LEU:HB2	53:3W:55:HIS:ND1	2.37	0.40
69:3W:101:3PE:C3	69:3W:101:3PE:P	3.09	0.40
75:3Y:106:CDL:H342	75:3Y:106:CDL:H311	1.77	0.40
55:4A:58:VAL:HG12	88:4A:601:HEA:HBD2	2.04	0.40
91:4A:609:PGV:C01	66:4L:28:TYR:HH	2.29	0.40
56:4B:98:LYS:HB2	56:4B:98:LYS:HE3	1.61	0.40
56:4B:198:GLU:O	56:4B:204:HIS:CE1	2.74	0.40
57:4C:187:THR:HA	87:4G:103:PEK:C04	2.51	0.40
63:4I:21:ILE:HD13	63:4I:21:ILE:HA	1.83	0.40
1:1A:104:TYR:HB2	69:1A:203:3PE:H371	2.03	0.40
6:1F:21:ILE:H	6:1F:21:ILE:HG13	1.69	0.40
6:1F:254:LYS:HD3	6:1F:332:ALA:HB2	2.03	0.40
6:1F:299:PRO:HG3	6:1F:327:THR:HG21	2.03	0.40
9:1I:52:PHE:O	42:1q:61:TRP:HA	2.21	0.40
9:1I:70:TYR:CZ	9:1I:76:ARG:HG2	2.56	0.40
9:1I:161:TRP:CE3	42:1q:84:PRO:HB3	2.57	0.40
10:1J:84:VAL:HA	10:1J:90:PHE:CZ	2.56	0.40
12:1L:7:LEU:O	12:1L:11:THR:HG23	2.21	0.40
69:1L:701:3PE:H3A2	69:1L:701:3PE:H372	1.89	0.40
69:1L:703:3PE:H2A1	69:1L:703:3PE:H2D2	1.94	0.40
69:1L:705:3PE:H3F2	82:1Y:203:PGT:H451	2.02	0.40
13:1M:24:TRP:CD2	13:1M:81:GLN:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:95:MET:HE3	14:1N:99:THR:OG1	2.21	0.40
75:1N:402:CDL:HB21	69:1e:201:3PE:O12	2.21	0.40
15:1O:318:TRP:CD1	15:1O:318:TRP:N	2.90	0.40
16:1P:95:VAL:HG23	79:1P:501:NDP:C4A	2.51	0.40
21:1V:85:ASN:HD22	21:1V:85:ASN:HA	1.63	0.40
24:1Y:62:SER:OG	69:1Y:208:3PE:H371	2.11	0.40
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.51	0.40
69:1d:201:3PE:H221	69:1d:201:3PE:H251	1.94	0.40
32:1g:109:GLU:O	41:1p:141:ARG:NH1	2.51	0.40
41:1p:72:ASP:OD1	41:1p:90:GLN:NE2	2.54	0.40
75:3A:501:CDL:H522	69:3A:503:3PE:C28	2.51	0.40
75:3A:501:CDL:OA7	69:3A:502:3PE:H11	2.21	0.40
46:3B:124:LEU:CD1	46:3B:224:LEU:HG	2.52	0.40
47:3C:62:ALA:O	47:3C:66:VAL:HG23	2.21	0.40
47:3C:109:PHE:CB	47:3C:112:THR:HG23	2.51	0.40
48:3D:294:GLY:HA2	48:3D:297:MET:HE3	2.03	0.40
49:3E:172:LYS:HG3	47:3P:262:LEU:CD2	2.51	0.40
50:3F:25:LEU:C	50:3F:27:GLY:N	2.70	0.40
46:3O:45:SER:CB	46:3O:116:ILE:CG1	3.00	0.40
70:3P:509:PC1:H3F1	70:3P:509:PC1:H3C2	1.77	0.40
75:3P:513:CDL:H451	69:3P:520:3PE:H352	2.04	0.40
48:3Q:11:PRO:HD3	52:3U:70:ALA:O	2.21	0.40
48:3Q:158:ILE:HG12	48:3Q:160:MET:H	1.86	0.40
69:3Q:502:3PE:H3B1	69:3Q:503:3PE:H2B2	2.04	0.40
49:3R:133:VAL:CG1	69:3R:304:3PE:H3B2	2.51	0.40
49:3R:197:ASP:H	49:3R:248:ARG:HH22	1.70	0.40
49:3R:211:VAL:HG21	49:3R:246:SER:HA	2.03	0.40
49:3R:253:PRO:HD2	72:3R:301:FES:S1	2.62	0.40
75:3T:101:CDL:C12	75:3T:101:CDL:H512	2.52	0.40
69:3T:103:3PE:H2C1	69:3T:103:3PE:H2F2	1.73	0.40
75:3X:103:CDL:H312	75:3X:103:CDL:HA31	2.03	0.40
69:3X:108:3PE:C39	69:4G:104:3PE:H392	2.50	0.40
57:4C:63:ARG:HA	57:4C:67:PHE:CD2	2.57	0.40
57:4C:104:SER:HA	91:4C:303:PGV:O06	2.21	0.40
58:4D:64:PHE:CD1	59:4E:66:ARG:HD3	2.57	0.40
91:4J:101:PGV:H311	91:4J:101:PGV:H281	1.92	0.40
2:1B:94:ASN:HB3	3:1C:174:LEU:HD22	2.03	0.40
69:1B:204:3PE:H241	69:1B:204:3PE:H272	1.81	0.40
5:1E:31:ILE:HG13	5:1E:53:LEU:HD23	2.03	0.40
5:1E:53:LEU:HD13	44:1s:52:LEU:HG	2.03	0.40
6:1F:140:GLY:O	6:1F:179:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:211:ALA:O	6:1F:219:PRO:HB3	2.22	0.40
6:1F:382:GLY:HA2	6:1F:430:MET:HG2	2.03	0.40
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.54	0.40
8:1H:176:PHE:O	25:1Z:46:GLY:HA3	2.20	0.40
9:1I:7:MET:HE2	9:1I:7:MET:HB3	1.88	0.40
69:1J:201:3PE:H3C1	69:1J:203:3PE:H281	2.02	0.40
12:1L:49:VAL:HB	12:1L:50:PRO:HD3	2.03	0.40
12:1L:63:ILE:HG13	34:1i:96:VAL:HG22	2.02	0.40
12:1L:142:ILE:HG21	75:1L:704:CDL:H822	2.03	0.40
12:1L:578:SER:HB2	14:1N:168:GLY:HA2	2.02	0.40
13:1M:319:HIS:HA	13:1M:322:THR:HG22	2.04	0.40
14:1N:263:LYS:HB3	14:1N:263:LYS:HE3	1.69	0.40
16:1P:248:VAL:O	16:1P:322:ARG:HD3	2.22	0.40
17:1Q:82:LEU:HD23	17:1Q:82:LEU:HA	1.81	0.40
24:1Y:38:TYR:HB3	69:1Y:204:3PE:C21	2.52	0.40
69:1Y:209:3PE:H291	75:3P:513:CDL:H871	2.03	0.40
69:1Y:216:3PE:H371	69:1Y:216:3PE:H3A1	1.86	0.40
75:1Y:217:CDL:H161	70:3T:102:PC1:O32	2.21	0.40
75:1Y:217:CDL:H341	75:1Y:217:CDL:H372	1.83	0.40
28:1c:23:THR:HG21	75:1d:205:CDL:H732	2.02	0.40
75:1g:201:CDL:H142	75:1g:201:CDL:C33	2.44	0.40
39:1n:62:LEU:HD23	39:1n:62:LEU:HA	1.79	0.40
75:3A:501:CDL:H772	69:3A:502:3PE:H2E2	2.04	0.40
47:3C:77:TRP:CE2	47:3C:78:VAL:HG12	2.56	0.40
69:3C:514:3PE:H261	69:3C:514:3PE:C38	2.49	0.40
48:3D:305:LEU:HB2	48:3D:306:PRO:HD3	2.02	0.40
52:3H:58:ALA:HA	52:3H:61:ARG:CZ	2.50	0.40
53:3J:39:GLY:HA3	69:3J:104:3PE:H3A2	2.04	0.40
70:3J:106:PC1:H112	70:3J:106:PC1:H133	1.68	0.40
45:3N:379:ILE:HG12	45:3N:389:ARG:HD3	2.03	0.40
69:3N:503:3PE:H3I3	69:3R:304:3PE:H3H1	2.04	0.40
46:3O:40:ASN:OD1	46:3O:40:ASN:N	2.45	0.40
46:3O:279:LEU:HD22	46:3O:295:LEU:HG	2.03	0.40
69:3P:514:3PE:H3F1	69:3P:514:3PE:H2C1	2.03	0.40
48:3Q:69:GLU:HG2	48:3Q:82:MET:HB3	2.03	0.40
48:3Q:70:VAL:HG12	48:3Q:71:GLN:N	2.36	0.40
48:3Q:139:THR:HG22	52:3U:44:VAL:CG1	2.52	0.40
49:3R:130:LYS:HA	69:3R:304:3PE:H282	2.04	0.40
49:3R:233:GLY:H	49:3R:244:ASP:C	2.30	0.40
49:3R:264:GLU:CB	49:3R:272:ILE:HG12	2.50	0.40
50:3S:52:GLU:OE2	51:3T:11:ARG:NH1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:4A:1:FME:HE2	55:4A:1:FME:HB2	1.95	0.40
55:4A:483:SER:HB3	67:4M:4:LYS:HG3	2.03	0.40
59:4E:7:THR:HB	59:4E:9:GLU:OE1	2.21	0.40
65:4K:31:TYR:O	65:4K:35:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	101 (89%)	9 (8%)	3 (3%)	4	1
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	198 (96%)	9 (4%)	0	100	100
4	1D	427/466 (92%)	411 (96%)	16 (4%)	0	100	100
5	1E	212/249 (85%)	198 (93%)	12 (6%)	2 (1%)	14	10
6	1F	430/464 (93%)	404 (94%)	22 (5%)	4 (1%)	14	10
7	1G	697/727 (96%)	667 (96%)	27 (4%)	3 (0%)	30	28
8	1H	316/318 (99%)	297 (94%)	17 (5%)	2 (1%)	21	18
9	1I	174/239 (73%)	167 (96%)	7 (4%)	0	100	100
10	1J	172/175 (98%)	160 (93%)	11 (6%)	1 (1%)	21	18
11	1K	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
12	1L	604/606 (100%)	567 (94%)	33 (6%)	4 (1%)	18	15
13	1M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
14	1N	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	36	36
15	1O	318/357 (89%)	296 (93%)	17 (5%)	5 (2%)	7	4
16	1P	340/377 (90%)	328 (96%)	11 (3%)	1 (0%)	36	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	81 (98%)	2 (2%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	21	18
24	1Y	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
25	1Z	139/144 (96%)	135 (97%)	4 (3%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	53 (96%)	2 (4%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	10 (10%)	0	100	100
33	1h	136/189 (72%)	133 (98%)	3 (2%)	0	100	100
34	1i	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	164 (96%)	6 (4%)	0	100	100
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	170 (99%)	1 (1%)	0	100	100
42	1q	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
43	1r	90/113 (80%)	84 (93%)	6 (7%)	0	100	100
44	1s	43/471 (9%)	40 (93%)	3 (7%)	0	100	100
45	3A	436/480 (91%)	418 (96%)	13 (3%)	5 (1%)	11	8
45	3N	444/480 (92%)	426 (96%)	12 (3%)	6 (1%)	9	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	3B	414/453 (91%)	387 (94%)	21 (5%)	6 (1%)	9	5
46	3O	413/453 (91%)	393 (95%)	19 (5%)	1 (0%)	43	44
47	3C	377/379 (100%)	368 (98%)	8 (2%)	1 (0%)	36	36
47	3P	377/379 (100%)	367 (97%)	9 (2%)	1 (0%)	36	36
48	3D	235/326 (72%)	228 (97%)	6 (3%)	1 (0%)	30	28
48	3Q	237/326 (73%)	224 (94%)	12 (5%)	1 (0%)	30	28
49	3E	194/274 (71%)	166 (86%)	18 (9%)	10 (5%)	1	0
49	3I	45/274 (16%)	31 (69%)	12 (27%)	2 (4%)	2	0
49	3R	194/274 (71%)	163 (84%)	22 (11%)	9 (5%)	2	0
49	3V	29/274 (11%)	28 (97%)	1 (3%)	0	100	100
50	3F	96/111 (86%)	92 (96%)	4 (4%)	0	100	100
50	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
51	3G	70/82 (85%)	69 (99%)	1 (1%)	0	100	100
51	3T	72/82 (88%)	71 (99%)	1 (1%)	0	100	100
52	3H	61/91 (67%)	60 (98%)	1 (2%)	0	100	100
52	3U	63/91 (69%)	62 (98%)	1 (2%)	0	100	100
53	3J	54/64 (84%)	50 (93%)	2 (4%)	2 (4%)	2	1
53	3W	52/64 (81%)	50 (96%)	1 (2%)	1 (2%)	6	3
54	3X	50/56 (89%)	46 (92%)	3 (6%)	1 (2%)	6	2
54	3Y	49/56 (88%)	45 (92%)	3 (6%)	1 (2%)	6	2
55	4A	512/514 (100%)	488 (95%)	21 (4%)	3 (1%)	21	18
56	4B	225/229 (98%)	211 (94%)	14 (6%)	0	100	100
57	4C	257/261 (98%)	245 (95%)	12 (5%)	0	100	100
58	4D	137/169 (81%)	126 (92%)	11 (8%)	0	100	100
59	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
60	4F	95/129 (74%)	90 (95%)	5 (5%)	0	100	100
61	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
62	4H	80/86 (93%)	72 (90%)	8 (10%)	0	100	100
63	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
64	4J	56/80 (70%)	54 (96%)	2 (4%)	0	100	100
65	4K	47/80 (59%)	44 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
66	4L	44/63 (70%)	42 (96%)	2 (4%)	0	100	100
67	4M	41/70 (59%)	41 (100%)	0	0	100	100
68	4N	80/82 (98%)	67 (84%)	13 (16%)	0	100	100
All	All	14068/16999 (83%)	13360 (95%)	630 (4%)	78 (1%)	23	18

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	115	ASP
8	1H	92	PRO
10	1J	66	VAL
12	1L	562	LEU
15	1O	138	MET
16	1P	276	GLU
23	1X	28	ALA
45	3A	369	LEU
46	3B	226	MET
46	3B	250	ASP
46	3B	309	VAL
49	3E	157	SER
49	3E	228	ALA
49	3E	271	VAL
53	3J	57	LYS
45	3N	71	PRO
45	3N	172	GLU
45	3N	224	VAL
49	3R	182	LYS
49	3R	228	ALA
53	3W	59	LYS
54	3X	46	PRO
54	3Y	46	PRO
1	1A	23	TRP
6	1F	205	LEU
8	1H	208	VAL
12	1L	601	LEU
15	1O	35	LYS
15	1O	137	ALA
45	3A	220	SER
45	3A	287	GLY
46	3B	288	GLY
48	3D	161	GLY

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Mol	Chain	Res	Type
49	3E	253	PRO
49	3E	256	LEU
49	3E	273	VAL
53	3J	54	LYS
45	3N	72	GLY
45	3N	214	LYS
48	3Q	73	GLY
49	3R	151	LYS
49	3R	229	GLY
49	3R	247	GLY
49	3R	273	VAL
55	4A	290	HIS
1	1A	52	SER
1	1A	109	LYS
6	1F	249	ARG
6	1F	297	VAL
12	1L	600	THR
15	1O	126	ARG
45	3A	350	THR
46	3B	289	SER
49	3E	142	ALA
49	3E	222	CYS
5	1E	110	LEU
5	1E	157	ASN
49	3E	223	VAL
49	3I	41	PRO
49	3I	56	SER
45	3N	287	GLY
46	3O	171	ALA
7	1G	654	GLN
15	1O	305	SER
45	3A	231	PHE
49	3E	267	SER
47	3P	221	HIS
6	1F	207	PRO
46	3B	248	ASN
49	3R	223	VAL
55	4A	128	VAL
7	1G	111	GLY
47	3C	221	HIS
55	4A	3	VAL
12	1L	2	ASN

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Mol	Chain	Res	Type
14	1N	110	PRO
49	3R	208	PRO
49	3R	237	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	92 (93%)	7 (7%)	13	11
2	1B	131/212 (62%)	121 (92%)	10 (8%)	12	9
3	1C	190/227 (84%)	186 (98%)	4 (2%)	47	54
4	1D	371/396 (94%)	357 (96%)	14 (4%)	29	32
5	1E	183/207 (88%)	177 (97%)	6 (3%)	33	37
6	1F	346/368 (94%)	332 (96%)	14 (4%)	28	29
7	1G	588/610 (96%)	556 (95%)	32 (5%)	20	18
8	1H	274/274 (100%)	267 (97%)	7 (3%)	40	46
9	1I	151/201 (75%)	143 (95%)	8 (5%)	20	19
10	1J	140/141 (99%)	126 (90%)	14 (10%)	7	5
11	1K	84/84 (100%)	80 (95%)	4 (5%)	23	23
12	1L	539/539 (100%)	510 (95%)	29 (5%)	20	18
13	1M	408/408 (100%)	388 (95%)	20 (5%)	22	22
14	1N	310/310 (100%)	294 (95%)	16 (5%)	21	20
15	1O	283/307 (92%)	266 (94%)	17 (6%)	17	15
16	1P	296/323 (92%)	280 (95%)	16 (5%)	20	18
17	1Q	117/152 (77%)	106 (91%)	11 (9%)	8	6
18	1R	79/97 (81%)	75 (95%)	4 (5%)	21	21
19	1S	77/82 (94%)	72 (94%)	5 (6%)	15	13
20	1T	79/133 (59%)	76 (96%)	3 (4%)	29	32
20	1U	79/133 (59%)	76 (96%)	3 (4%)	29	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1V	100/101 (99%)	95 (95%)	5 (5%)	22	22
22	1W	107/112 (96%)	104 (97%)	3 (3%)	38	43
23	1X	153/154 (99%)	146 (95%)	7 (5%)	24	25
24	1Y	101/102 (99%)	93 (92%)	8 (8%)	11	9
25	1Z	123/124 (99%)	120 (98%)	3 (2%)	43	49
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	35
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	11
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	12
29	1d	106/109 (97%)	100 (94%)	6 (6%)	18	17
30	1e	87/94 (93%)	83 (95%)	4 (5%)	24	25
31	1f	54/113 (48%)	49 (91%)	5 (9%)	8	6
32	1g	92/129 (71%)	90 (98%)	2 (2%)	45	53
33	1h	121/158 (77%)	117 (97%)	4 (3%)	33	37
34	1i	120/120 (100%)	116 (97%)	4 (3%)	33	37
35	1j	62/84 (74%)	57 (92%)	5 (8%)	11	8
36	1k	63/76 (83%)	59 (94%)	4 (6%)	16	14
37	1l	141/161 (88%)	137 (97%)	4 (3%)	38	43
38	1m	113/114 (99%)	109 (96%)	4 (4%)	32	35
39	1n	156/160 (98%)	148 (95%)	8 (5%)	21	21
40	1o	110/119 (92%)	106 (96%)	4 (4%)	31	34
41	1p	154/156 (99%)	152 (99%)	2 (1%)	61	69
42	1q	131/131 (100%)	128 (98%)	3 (2%)	44	51
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32	35
44	1s	44/351 (12%)	42 (96%)	2 (4%)	24	25
45	3A	367/397 (92%)	354 (96%)	13 (4%)	32	35
45	3N	372/397 (94%)	350 (94%)	22 (6%)	18	16
46	3B	328/355 (92%)	314 (96%)	14 (4%)	26	27
46	3O	327/355 (92%)	313 (96%)	14 (4%)	26	27
47	3C	332/332 (100%)	320 (96%)	12 (4%)	31	34
47	3P	332/332 (100%)	318 (96%)	14 (4%)	26	28
48	3D	202/259 (78%)	190 (94%)	12 (6%)	18	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	3Q	204/259 (79%)	195 (96%)	9 (4%)	25	26
49	3E	166/225 (74%)	146 (88%)	20 (12%)	5	3
49	3I	36/225 (16%)	27 (75%)	9 (25%)	0	0
49	3R	166/225 (74%)	144 (87%)	22 (13%)	4	2
49	3V	24/225 (11%)	21 (88%)	3 (12%)	4	2
50	3F	90/99 (91%)	89 (99%)	1 (1%)	65	74
50	3S	90/99 (91%)	89 (99%)	1 (1%)	65	74
51	3G	67/73 (92%)	63 (94%)	4 (6%)	17	15
51	3T	67/73 (92%)	63 (94%)	4 (6%)	17	15
52	3H	62/85 (73%)	59 (95%)	3 (5%)	23	23
52	3U	62/85 (73%)	55 (89%)	7 (11%)	5	3
53	3J	46/52 (88%)	45 (98%)	1 (2%)	45	53
53	3W	46/52 (88%)	44 (96%)	2 (4%)	26	27
54	3X	42/46 (91%)	42 (100%)	0	100	100
54	3Y	41/46 (89%)	40 (98%)	1 (2%)	43	49
55	4A	424/424 (100%)	417 (98%)	7 (2%)	53	62
56	4B	210/211 (100%)	201 (96%)	9 (4%)	26	27
57	4C	223/225 (99%)	216 (97%)	7 (3%)	35	39
58	4D	124/149 (83%)	119 (96%)	5 (4%)	28	29
59	4E	92/124 (74%)	90 (98%)	2 (2%)	45	53
60	4F	80/101 (79%)	76 (95%)	4 (5%)	22	22
61	4G	65/80 (81%)	59 (91%)	6 (9%)	8	6
62	4H	73/76 (96%)	71 (97%)	2 (3%)	39	45
63	4I	54/61 (88%)	50 (93%)	4 (7%)	13	10
64	4J	49/68 (72%)	49 (100%)	0	100	100
65	4K	38/66 (58%)	36 (95%)	2 (5%)	20	19
66	4L	39/55 (71%)	38 (97%)	1 (3%)	40	46
67	4M	37/57 (65%)	35 (95%)	2 (5%)	20	18
68	4N	70/70 (100%)	67 (96%)	3 (4%)	26	27
All	All	12266/14326 (86%)	11680 (95%)	586 (5%)	24	23

All (586) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	6	THR
1	1A	8	LEU
1	1A	16	LEU
1	1A	23	TRP
1	1A	54	LYS
1	1A	57	LEU
1	1A	115	GLU
2	1B	30	VAL
2	1B	32	LYS
2	1B	34	ASP
2	1B	54	CYS
2	1B	61	HIS
2	1B	85	VAL
2	1B	91	THR
2	1B	106	GLN
2	1B	125	TYR
2	1B	137	ASP
3	1C	62	THR
3	1C	114	LEU
3	1C	117	ILE
3	1C	177	ASP
4	1D	61	VAL
4	1D	68	LEU
4	1D	85	ARG
4	1D	109	VAL
4	1D	125	LEU
4	1D	128	ILE
4	1D	140	LEU
4	1D	219	SER
4	1D	225	LEU
4	1D	252	ASN
4	1D	281	VAL
4	1D	282	GLU
4	1D	342	MET
4	1D	424	VAL
5	1E	75	VAL
5	1E	89	MET
5	1E	110	LEU
5	1E	149	VAL
5	1E	181	ILE
5	1E	199	LEU
6	1F	10	THR
6	1F	94	VAL

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Mol	Chain	Res	Type
6	1F	104	THR
6	1F	110	ILE
6	1F	114	ASP
6	1F	151	VAL
6	1F	175	VAL
6	1F	188	GLU
6	1F	213	VAL
6	1F	250	ASN
6	1F	287	VAL
6	1F	336	VAL
6	1F	404	ILE
6	1F	415	VAL
7	1G	56	LEU
7	1G	65	VAL
7	1G	77	TRP
7	1G	93	VAL
7	1G	98	LEU
7	1G	116	LEU
7	1G	117	GLN
7	1G	137	VAL
7	1G	146	VAL
7	1G	151	THR
7	1G	172	LEU
7	1G	180	ASP
7	1G	199	ILE
7	1G	205	VAL
7	1G	210	SER
7	1G	225	THR
7	1G	242	THR
7	1G	323	VAL
7	1G	329	VAL
7	1G	348	VAL
7	1G	351	THR
7	1G	360	SER
7	1G	366	THR
7	1G	371	VAL
7	1G	402	ASN
7	1G	471	SER
7	1G	517	ASN
7	1G	531	CYS
7	1G	585	VAL
7	1G	600	ILE

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Mol	Chain	Res	Type
7	1G	636	VAL
7	1G	703	ILE
8	1H	87	VAL
8	1H	102	VAL
8	1H	119	SER
8	1H	178	SER
8	1H	271	LEU
8	1H	285	LEU
8	1H	296	LEU
9	1I	5	VAL
9	1I	34	LEU
9	1I	37	THR
9	1I	41	LEU
9	1I	78	ILE
9	1I	107	THR
9	1I	122	CYS
9	1I	129	ASP
10	1J	4	TYR
10	1J	33	LEU
10	1J	34	ILE
10	1J	41	CYS
10	1J	50	SER
10	1J	57	PHE
10	1J	61	LEU
10	1J	76	THR
10	1J	97	LEU
10	1J	99	MET
10	1J	103	MET
10	1J	113	VAL
10	1J	163	ILE
10	1J	172	THR
11	1K	14	ILE
11	1K	26	LEU
11	1K	29	SER
11	1K	91	GLN
12	1L	8	THR
12	1L	36	VAL
12	1L	38	THR
12	1L	46	LEU
12	1L	57	THR
12	1L	69	MET
12	1L	73	THR

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Mol	Chain	Res	Type
12	1L	100	ILE
12	1L	114	ILE
12	1L	140	LEU
12	1L	149	ILE
12	1L	162	THR
12	1L	206	ASN
12	1L	277	THR
12	1L	296	ASN
12	1L	307	SER
12	1L	371	THR
12	1L	387	THR
12	1L	417	SER
12	1L	447	ASN
12	1L	484	LEU
12	1L	489	THR
12	1L	491	LEU
12	1L	500	LEU
12	1L	507	THR
12	1L	531	SER
12	1L	566	THR
12	1L	572	LYS
12	1L	592	LEU
13	1M	9	THR
13	1M	36	LEU
13	1M	55	THR
13	1M	57	PHE
13	1M	58	SER
13	1M	60	SER
13	1M	70	THR
13	1M	88	THR
13	1M	94	LEU
13	1M	116	ILE
13	1M	122	PHE
13	1M	140	THR
13	1M	205	VAL
13	1M	214	LEU
13	1M	340	ARG
13	1M	343	ILE
13	1M	369	LEU
13	1M	375	LEU
13	1M	393	ILE
13	1M	429	SER

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Mol	Chain	Res	Type
14	1N	43	VAL
14	1N	70	LEU
14	1N	85	THR
14	1N	93	VAL
14	1N	100	MET
14	1N	115	VAL
14	1N	170	LEU
14	1N	173	THR
14	1N	182	SER
14	1N	222	SER
14	1N	250	SER
14	1N	282	MET
14	1N	301	SER
14	1N	336	VAL
14	1N	343	LEU
14	1N	344	SER
15	1O	6	LEU
15	1O	14	THR
15	1O	18	LEU
15	1O	24	VAL
15	1O	60	ASP
15	1O	67	LYS
15	1O	88	SER
15	1O	96	LEU
15	1O	115	LEU
15	1O	122	VAL
15	1O	195	THR
15	1O	215	SER
15	1O	220	VAL
15	1O	222	GLN
15	1O	230	ASP
15	1O	232	GLU
15	1O	263	VAL
16	1P	20	VAL
16	1P	43	SER
16	1P	81	ILE
16	1P	83	LYS
16	1P	90	VAL
16	1P	108	ASP
16	1P	126	VAL
16	1P	141	SER
16	1P	143	SER

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Mol	Chain	Res	Type
16	1P	148	SER
16	1P	191	VAL
16	1P	231	VAL
16	1P	241	LEU
16	1P	263	TYR
16	1P	315	ILE
16	1P	340	VAL
17	1Q	14	ASP
17	1Q	22	LEU
17	1Q	27	GLU
17	1Q	33	ARG
17	1Q	44	ASN
17	1Q	61	THR
17	1Q	77	ASP
17	1Q	79	LEU
17	1Q	82	LEU
17	1Q	105	VAL
17	1Q	115	SER
18	1R	24	ARG
18	1R	71	VAL
18	1R	78	GLU
18	1R	83	THR
19	1S	13	LEU
19	1S	20	ILE
19	1S	64	LEU
19	1S	76	VAL
19	1S	77	SER
20	1T	30	LEU
20	1T	31	SER
20	1T	40	LEU
20	1U	31	SER
20	1U	64	ASP
20	1U	77	VAL
21	1V	8	THR
21	1V	13	LEU
21	1V	22	ARG
21	1V	102	LEU
21	1V	103	VAL
22	1W	74	THR
22	1W	96	VAL
22	1W	101	THR
23	1X	12	LEU

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Mol	Chain	Res	Type
23	1X	17	VAL
23	1X	41	GLU
23	1X	97	ARG
23	1X	99	CYS
23	1X	111	LEU
23	1X	130	VAL
24	1Y	4	LEU
24	1Y	11	ILE
24	1Y	25	THR
24	1Y	31	THR
24	1Y	35	VAL
24	1Y	39	SER
24	1Y	47	SER
24	1Y	76	SER
25	1Z	124	LEU
25	1Z	133	ILE
25	1Z	135	SER
26	1a	1	MET
26	1a	57	VAL
27	1b	19	VAL
27	1b	34	LEU
27	1b	65	VAL
27	1b	76	SER
27	1b	83	LEU
28	1c	21	LEU
28	1c	24	SER
28	1c	49	GLU
29	1d	41	SER
29	1d	43	LEU
29	1d	53	VAL
29	1d	55	SER
29	1d	62	LEU
29	1d	111	GLU
30	1e	5	VAL
30	1e	57	ILE
30	1e	92	THR
30	1e	98	LEU
31	1f	5	GLN
31	1f	25	TYR
31	1f	33	LYS
31	1f	51	ASN
31	1f	54	VAL

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Mol	Chain	Res	Type
32	1g	43	ASP
32	1g	70	LEU
33	1h	24	LEU
33	1h	57	GLU
33	1h	102	GLU
33	1h	113	LEU
34	1i	38	ARG
34	1i	47	ASN
34	1i	67	SER
34	1i	90	THR
35	1j	23	ILE
35	1j	29	SER
35	1j	50	HIS
35	1j	63	GLU
35	1j	70	ASP
36	1k	19	LYS
36	1k	32	GLN
36	1k	81	VAL
36	1k	87	LEU
37	1l	5	THR
37	1l	81	LEU
37	1l	92	SER
37	1l	147	THR
38	1m	24	ILE
38	1m	87	LEU
38	1m	123	THR
38	1m	127	SER
39	1n	8	TYR
39	1n	26	LEU
39	1n	88	THR
39	1n	89	SER
39	1n	109	SER
39	1n	157	ARG
39	1n	162	LEU
39	1n	169	ILE
40	1o	9	LEU
40	1o	19	LEU
40	1o	23	THR
40	1o	54	GLN
41	1p	139	GLN
41	1p	167	LYS
42	1q	3	LEU

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Mol	Chain	Res	Type
42	1q	32	ASP
42	1q	129	THR
43	1r	11	ARG
43	1r	23	LEU
43	1r	26	ARG
44	1s	48	THR
44	1s	61	PHE
45	3A	45	SER
45	3A	49	ASN
45	3A	51	LYS
45	3A	52	ASN
45	3A	61	HIS
45	3A	86	LEU
45	3A	108	LYS
45	3A	176	LYS
45	3A	214	LYS
45	3A	219	LEU
45	3A	281	ASP
45	3A	308	GLN
45	3A	350	THR
46	3B	95	LYS
46	3B	117	GLU
46	3B	119	LEU
46	3B	200	THR
46	3B	212	SER
46	3B	221	GLU
46	3B	252	LEU
46	3B	297	GLN
46	3B	301	LYS
46	3B	309	VAL
46	3B	315	SER
46	3B	338	LYS
46	3B	436	VAL
46	3B	438	GLU
47	3C	18	PHE
47	3C	78	VAL
47	3C	112	THR
47	3C	160	LEU
47	3C	174	THR
47	3C	202	GLU
47	3C	215	MET
47	3C	269	LYS

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Mol	Chain	Res	Type
47	3C	281	LEU
47	3C	284	ILE
47	3C	306	MET
47	3C	344	GLU
48	3D	125	CYS
48	3D	126	SER
48	3D	150	LYS
48	3D	154	GLU
48	3D	165	ASP
48	3D	185	ASN
48	3D	227	THR
48	3D	229	VAL
48	3D	231	LEU
48	3D	232	ARG
48	3D	258	LEU
48	3D	262	ASP
49	3E	83	ILE
49	3E	155	LYS
49	3E	172	LYS
49	3E	177	ARG
49	3E	180	THR
49	3E	181	LYS
49	3E	182	LYS
49	3E	184	ILE
49	3E	186	GLN
49	3E	194	GLN
49	3E	195	LEU
49	3E	204	ARG
49	3E	205	VAL
49	3E	209	GLU
49	3E	211	VAL
49	3E	212	ILE
49	3E	213	LEU
49	3E	222	CYS
49	3E	257	ASN
49	3E	271	VAL
50	3F	26	GLU
51	3G	48	LEU
51	3G	72	LYS
51	3G	74	LYS
51	3G	75	ASN
52	3H	60	GLU

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Mol	Chain	Res	Type
52	3H	64	LEU
52	3H	73	SER
49	3I	34	LEU
49	3I	39	GLU
49	3I	47	ARG
49	3I	50	LEU
49	3I	55	LEU
49	3I	70	LEU
49	3I	72	VAL
49	3I	76	VAL
49	3I	77	ARG
53	3J	10	LEU
45	3N	24	ARG
45	3N	30	SER
45	3N	32	GLN
45	3N	41	ILE
45	3N	49	ASN
45	3N	61	HIS
45	3N	67	THR
45	3N	69	ASN
45	3N	112	LEU
45	3N	117	VAL
45	3N	148	VAL
45	3N	149	VAL
45	3N	172	GLU
45	3N	219	LEU
45	3N	224	VAL
45	3N	228	VAL
45	3N	303	LEU
45	3N	308	GLN
45	3N	348	SER
45	3N	402	VAL
45	3N	403	ASP
45	3N	444	LEU
46	3O	29	LEU
46	3O	31	ASN
46	3O	69	LEU
46	3O	71	LEU
46	3O	74	SER
46	3O	95	LYS
46	3O	110	GLU
46	3O	116	ILE

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Mol	Chain	Res	Type
46	3O	117	GLU
46	3O	209	LEU
46	3O	211	VAL
46	3O	212	SER
46	3O	222	ARG
46	3O	232	LEU
47	3P	1	MET
47	3P	13	ILE
47	3P	14	ILE
47	3P	108	MET
47	3P	112	THR
47	3P	146	ILE
47	3P	150	LEU
47	3P	174	THR
47	3P	197	LEU
47	3P	281	LEU
47	3P	284	ILE
47	3P	287	LYS
47	3P	304	MET
47	3P	306	MET
48	3Q	3	LEU
48	3Q	21	LEU
48	3Q	34	LYS
48	3Q	37	CYS
48	3Q	68	VAL
48	3Q	77	ASP
48	3Q	86	LYS
48	3Q	169	LEU
48	3Q	214	LEU
49	3R	83	ILE
49	3R	90	ASP
49	3R	163	LYS
49	3R	168	LYS
49	3R	179	ARG
49	3R	180	THR
49	3R	185	ASP
49	3R	187	GLU
49	3R	196	ARG
49	3R	199	GLN
49	3R	203	GLU
49	3R	207	LYS
49	3R	213	LEU

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Mol	Chain	Res	Type
49	3R	214	ILE
49	3R	219	HIS
49	3R	234	TYR
49	3R	235	TYR
49	3R	251	LYS
49	3R	256	LEU
49	3R	263	TYR
49	3R	265	PHE
49	3R	271	VAL
50	3S	12	TRP
51	3T	7	LEU
51	3T	10	MET
51	3T	54	VAL
51	3T	71	ARG
52	3U	23	GLN
52	3U	25	GLU
52	3U	28	GLU
52	3U	39	LEU
52	3U	42	GLN
52	3U	68	CYS
52	3U	75	ASN
49	3V	55	LEU
49	3V	62	ARG
49	3V	64	LEU
53	3W	7	THR
53	3W	56	ILE
54	3Y	11	ARG
55	4A	75	ILE
55	4A	101	SER
55	4A	215	LEU
55	4A	307	SER
55	4A	357	VAL
55	4A	485	VAL
55	4A	489	SER
56	4B	54	SER
56	4B	73	LEU
56	4B	75	LEU
56	4B	87	MET
56	4B	107	SER
56	4B	115	ASP
56	4B	138	VAL
56	4B	142	VAL

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Mol	Chain	Res	Type
56	4B	220	GLU
57	4C	29	SER
57	4C	74	VAL
57	4C	132	LEU
57	4C	145	THR
57	4C	155	ASP
57	4C	192	VAL
57	4C	212	SER
58	4D	26	ASP
58	4D	33	LEU
58	4D	54	ASP
58	4D	87	PHE
58	4D	140	TYR
59	4E	36	LEU
59	4E	92	THR
60	4F	48	LEU
60	4F	63	GLU
60	4F	79	THR
60	4F	94	HIS
61	4G	15	THR
61	4G	30	LEU
61	4G	64	ASP
61	4G	69	LEU
61	4G	72	ASN
61	4G	75	VAL
62	4H	13	THR
62	4H	50	VAL
63	4I	21	ILE
63	4I	22	VAL
63	4I	44	LYS
63	4I	56	SER
65	4K	15	ASN
65	4K	20	SER
66	4L	4	GLU
67	4M	20	SER
67	4M	25	SER
68	4N	7	THR
68	4N	49	ASN
68	4N	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	162	GLN
2	1B	164	GLN
3	1C	39	GLN
3	1C	41	GLN
3	1C	95	ASN
3	1C	144	ASN
4	1D	232	ASN
4	1D	348	HIS
5	1E	16	ASN
6	1F	144	ASN
6	1F	200	GLN
6	1F	356	HIS
6	1F	361	GLN
6	1F	398	GLN
7	1G	100	ASN
7	1G	141	ASN
7	1G	155	GLN
7	1G	179	ASN
7	1G	237	ASN
7	1G	255	HIS
7	1G	259	ASN
7	1G	459	GLN
7	1G	476	ASN
7	1G	629	ASN
8	1H	47	GLN
8	1H	138	GLN
8	1H	235	ASN
10	1J	46	ASN
12	1L	30	ASN
12	1L	192	HIS
12	1L	194	ASN
12	1L	296	ASN
12	1L	323	HIS
12	1L	506	ASN
12	1L	524	ASN
12	1L	580	GLN
12	1L	603	ASN
13	1M	144	ASN
13	1M	331	ASN
13	1M	421	HIS
14	1N	152	ASN
14	1N	310	ASN
15	1O	30	ASN

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Mol	Chain	Res	Type
15	1O	57	HIS
15	1O	265	ASN
15	1O	288	GLN
15	1O	294	GLN
16	1P	341	ASN
18	1R	32	GLN
18	1R	95	HIS
19	1S	61	GLN
20	1T	35	HIS
20	1U	33	ASN
20	1U	74	GLN
21	1V	75	GLN
21	1V	82	GLN
22	1W	51	GLN
22	1W	99	GLN
22	1W	102	HIS
23	1X	34	GLN
23	1X	102	GLN
24	1Y	88	ASN
26	1a	46	ASN
28	1c	34	GLN
29	1d	46	ASN
30	1e	97	HIS
31	1f	5	GLN
36	1k	59	ASN
38	1m	32	GLN
38	1m	78	ASN
39	1n	77	GLN
41	1p	106	GLN
41	1p	123	ASN
41	1p	139	GLN
43	1r	12	ASN
43	1r	24	GLN
43	1r	35	GLN
44	1s	44	HIS
44	1s	65	GLN
45	3A	32	GLN
45	3A	49	ASN
45	3A	52	ASN
45	3A	69	ASN
45	3A	94	HIS
45	3A	118	GLN

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Mol	Chain	Res	Type
45	3A	136	GLN
45	3A	165	GLN
45	3A	243	HIS
45	3A	305	GLN
45	3A	363	ASN
45	3A	435	ASN
46	3B	22	GLN
46	3B	156	GLN
46	3B	247	GLN
46	3B	358	GLN
46	3B	394	GLN
46	3B	400	GLN
46	3B	429	ASN
47	3C	16	ASN
47	3C	32	ASN
47	3C	68	HIS
47	3C	97	HIS
47	3C	196	HIS
47	3C	201	HIS
47	3C	207	ASN
47	3C	286	ASN
47	3C	345	HIS
47	3C	352	GLN
47	3C	375	ASN
48	3D	102	HIS
48	3D	119	GLN
48	3D	163	ASN
48	3D	193	ASN
48	3D	238	ASN
49	3E	178	HIS
49	3E	186	GLN
49	3E	194	GLN
49	3E	200	HIS
50	3F	34	ASN
52	3H	51	GLN
52	3H	67	GLN
53	3J	46	HIS
53	3J	49	GLN
45	3N	9	GLN
45	3N	53	ASN
45	3N	94	HIS
45	3N	118	GLN

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Mol	Chain	Res	Type
46	3O	143	GLN
46	3O	158	GLN
46	3O	254	HIS
46	3O	290	ASN
46	3O	297	GLN
46	3O	305	GLN
46	3O	351	ASN
46	3O	354	ASN
46	3O	432	HIS
47	3P	8	HIS
47	3P	68	HIS
47	3P	85	ASN
47	3P	267	HIS
47	3P	341	GLN
48	3Q	31	GLN
48	3Q	35	GLN
48	3Q	105	ASN
48	3Q	181	GLN
49	3R	135	GLN
49	3R	200	HIS
49	3R	227	ASN
49	3R	239	HIS
49	3R	257	ASN
50	3S	22	ASN
51	3T	6	HIS
52	3U	23	GLN
52	3U	26	GLN
53	3W	58	HIS
55	4A	11	ASN
55	4A	232	GLN
55	4A	406	ASN
55	4A	407	GLN
55	4A	491	ASN
56	4B	24	HIS
56	4B	52	HIS
57	4C	12	ASN
57	4C	50	ASN
57	4C	133	ASN
57	4C	204	HIS
57	4C	243	HIS
58	4D	76	ASN
59	4E	20	ASN

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Mol	Chain	Res	Type
61	4G	51	HIS
62	4H	25	GLN
62	4H	32	ASN
63	4I	53	ASN
64	4J	16	ASN
65	4K	35	GLN
65	4K	41	ASN
66	4L	17	ASN
67	4M	39	HIS
68	4N	8	GLN
68	4N	49	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	FME	4B	1	56	8,9,10	0.54	0	8,9,11	0.89	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	0.84	1 (12%)
13	FME	1M	1	13	8,9,10	0.50	0	8,9,11	1.64	2 (25%)
1	FME	1A	1	1	8,9,10	0.50	0	8,9,11	1.10	1 (12%)
14	FME	1N	1	14	8,9,10	0.55	0	8,9,11	0.96	1 (12%)
55	FME	4A	1	55	8,9,10	0.55	0	8,9,11	1.73	2 (25%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.05	1 (12%)
11	FME	1K	1	11	8,9,10	0.57	0	8,9,11	0.97	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	FME	4B	1	56	-	2/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
13	FME	1M	1	13	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
55	FME	4A	1	55	-	1/7/9/11	-
8	FME	1H	1	8	-	2/7/9/11	-
11	FME	1K	1	11	-	2/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	4A	1	FME	CA-N-CN	3.85	128.74	122.82
13	1M	1	FME	O-C-CA	-2.98	117.11	124.77
13	1M	1	FME	CA-N-CN	-2.87	118.41	122.82
1	1A	1	FME	O-C-CA	-2.75	117.69	124.77
8	1H	1	FME	O-C-CA	-2.70	117.82	124.77
11	1K	1	FME	O-C-CA	-2.63	118.00	124.77
14	1N	1	FME	O-C-CA	-2.50	118.34	124.77
56	4B	1	FME	O-C-CA	-2.32	118.79	124.77
55	4A	1	FME	O-C-CA	-2.24	119.00	124.77
12	1L	1	FME	O-C-CA	-2.19	119.13	124.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O1-CN-N-CA
8	1H	1	FME	O1-CN-N-CA
13	1M	1	FME	C-CA-CB-CG
14	1N	1	FME	O1-CN-N-CA
56	4B	1	FME	O1-CN-N-CA
56	4B	1	FME	CB-CA-N-CN
55	4A	1	FME	CA-CB-CG-SD
11	1K	1	FME	C-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
13	1M	1	FME	N-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
8	1H	1	FME	CB-CA-N-CN

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1M	1	FME	5	0
1	1A	1	FME	1	0
14	1N	1	FME	1	0
55	4A	1	FME	7	0
11	1K	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 226 ligands modelled in this entry, 7 are monoatomic - leaving 219 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
69	3PE	3P	507	-	50,50,50	0.93	2 (4%)	53,55,55	1.11	3 (5%)
69	3PE	3R	304	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	3 (5%)
69	3PE	3E	303	-	48,48,50	0.90	3 (6%)	51,53,55	1.17	4 (7%)
70	PC1	1Y	207	-	53,53,53	0.93	2 (3%)	59,61,61	1.16	3 (5%)
75	CDL	3X	103	-	99,99,99	0.91	4 (4%)	105,111,111	1.11	5 (4%)
69	3PE	1L	708	-	41,41,50	0.99	2 (4%)	44,46,55	1.27	4 (9%)
69	3PE	3G	107	-	32,32,50	1.14	2 (6%)	35,37,55	1.12	2 (5%)
69	3PE	3X	107	-	50,50,50	0.91	2 (4%)	53,55,55	0.96	3 (5%)
69	3PE	3C	511	-	50,50,50	0.91	2 (4%)	53,55,55	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
75	CDL	1H	401	-	50,50,99	1.28	4 (8%)	56,62,111	1.31	7 (12%)
75	CDL	3T	101	-	56,56,99	1.18	6 (10%)	62,68,111	1.41	8 (12%)
81	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.06	1 (2%)
91	PGV	4C	303	-	50,50,50	0.89	2 (4%)	53,56,56	0.93	2 (3%)
69	3PE	3W	102	-	41,41,50	0.99	2 (4%)	44,46,55	1.05	2 (4%)
69	3PE	3N	501	-	50,50,50	0.89	3 (6%)	53,55,55	1.13	3 (5%)
72	FES	1E	301	5	0,4,4	-	-	-	-	-
69	3PE	3C	506	-	46,46,50	0.93	2 (4%)	49,51,55	1.14	4 (8%)
69	3PE	3J	102	-	37,37,50	1.06	2 (5%)	40,42,55	1.27	4 (10%)
69	3PE	3P	508	-	50,50,50	0.90	4 (8%)	53,55,55	1.33	7 (13%)
69	3PE	3N	503	-	50,50,50	0.91	3 (6%)	53,55,55	1.14	4 (7%)
94	PO4	4H	101	-	4,4,4	0.98	0	6,6,6	0.47	0
69	3PE	3P	510	-	47,47,50	0.92	2 (4%)	50,52,55	1.09	5 (10%)
75	CDL	4C	306	-	99,99,99	0.91	4 (4%)	105,111,111	1.05	6 (5%)
69	3PE	1A	203	-	40,40,50	1.01	2 (5%)	43,45,55	1.19	4 (9%)
69	3PE	1Y	211	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
91	PGV	4K	101	-	42,42,50	0.99	2 (4%)	45,48,56	1.11	3 (6%)
69	3PE	3G	103	-	32,32,50	1.12	2 (6%)	35,37,55	1.27	2 (5%)
69	3PE	1Y	208	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	3Q	502	-	40,40,50	1.02	2 (5%)	43,45,55	4.81	4 (9%)
71	SF4	1I	201	9	0,12,12	-	-	-	-	-
69	3PE	3E	302	-	50,50,50	0.87	2 (4%)	53,55,55	1.22	4 (7%)
70	PC1	1Y	206	-	45,45,53	1.00	2 (4%)	51,53,61	1.10	3 (5%)
69	3PE	3X	106	-	50,50,50	0.92	2 (4%)	53,55,55	0.97	2 (3%)
69	3PE	1Y	214	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	1Y	216	-	50,50,50	0.90	2 (4%)	53,55,55	1.15	5 (9%)
83	AME	1h	201	-	9,10,11	0.53	0	9,11,13	0.99	1 (11%)
93	PSC	4B	303	-	51,51,51	0.95	2 (3%)	57,59,59	1.02	4 (7%)
91	PGV	4A	607	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	3X	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.06	4 (7%)
85	HEM	3C	502	-	50,50,50	1.60	9 (18%)	67,82,82	1.62	15 (22%)
69	3PE	3C	507	-	50,50,50	0.94	2 (4%)	53,55,55	1.06	2 (3%)
69	3PE	1L	712	-	50,50,50	0.93	2 (4%)	53,55,55	1.09	2 (3%)
69	3PE	1l	203	-	32,32,50	1.14	2 (6%)	35,37,55	1.16	2 (5%)
69	3PE	3C	510	-	34,34,50	1.16	3 (8%)	37,39,55	1.88	5 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	3X	108	-	50,50,50	0.91	2 (4%)	53,55,55	1.00	2 (3%)
79	NDP	1P	501	-	51,52,52	0.51	0	71,80,80	0.82	2 (2%)
69	3PE	3P	517	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	1Y	205	-	39,39,50	1.05	2 (5%)	42,44,55	0.96	2 (4%)
69	3PE	1Y	201	-	41,41,50	1.00	2 (4%)	44,46,55	1.10	3 (6%)
84	MYR	1I	201	-	13,14,15	0.32	0	12,13,15	0.29	0
69	3PE	3S	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.02	2 (3%)
85	HEM	3P	502	47	50,50,50	1.61	9 (18%)	67,82,82	1.64	16 (23%)
69	3PE	3Q	503	-	45,45,50	0.99	2 (4%)	48,50,55	1.11	2 (4%)
76	AYA	1I	203	-	6,7,8	0.65	0	6,8,10	0.79	0
69	3PE	3C	503	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	4 (7%)
69	3PE	1L	705	-	48,48,50	0.91	2 (4%)	51,53,55	1.25	5 (9%)
75	CDL	3F	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.08	7 (6%)
86	HEC	3D	501	48	44,49,50	2.59	24 (54%)	56,80,82	2.10	18 (32%)
69	3PE	3P	516	-	50,50,50	0.91	2 (4%)	53,55,55	1.05	3 (5%)
69	3PE	3G	102	-	32,32,50	1.15	2 (6%)	35,37,55	1.08	2 (5%)
69	3PE	3R	302	-	50,50,50	0.87	3 (6%)	53,55,55	1.25	5 (9%)
69	3PE	1N	401	-	50,50,50	0.88	2 (4%)	53,55,55	1.24	5 (9%)
69	3PE	3C	514	-	34,34,50	1.05	2 (5%)	37,39,55	1.25	5 (13%)
81	EHZ	1T	101	20	31,36,37	0.20	0	36,44,47	1.11	1 (2%)
69	3PE	1I	204	-	50,50,50	0.93	2 (4%)	53,55,55	1.06	3 (5%)
69	3PE	3P	512	-	47,47,50	0.92	2 (4%)	50,52,55	1.10	3 (6%)
69	3PE	1L	706	-	32,32,50	1.16	2 (6%)	35,37,55	1.07	2 (5%)
70	PC1	1P	502	-	32,32,53	1.22	2 (6%)	38,40,61	1.11	4 (10%)
69	3PE	3G	110	-	42,42,50	0.97	2 (4%)	45,47,55	1.09	3 (6%)
69	3PE	1d	203	-	46,46,50	0.95	2 (4%)	49,51,55	1.12	3 (6%)
69	3PE	1m	202	-	41,41,50	0.99	2 (4%)	44,46,55	1.17	3 (6%)
88	HEA	4A	601	55	67,67,67	2.40	23 (34%)	81,103,103	2.55	35 (43%)
69	3PE	3G	109	-	50,50,50	0.90	2 (4%)	53,55,55	1.10	3 (5%)
69	3PE	1m	201	-	49,49,50	0.92	2 (4%)	52,54,55	1.07	2 (3%)
69	3PE	3P	504	-	37,37,50	1.06	2 (5%)	40,42,55	1.16	2 (5%)
69	3PE	1f	102	-	42,42,50	0.99	2 (4%)	45,47,55	1.07	3 (6%)
88	HEA	4A	602	55	67,67,67	2.42	22 (32%)	81,103,103	2.50	36 (44%)
70	PC1	1H	404	-	40,40,53	1.12	3 (7%)	46,48,61	1.29	6 (13%)
69	3PE	1Y	215	-	42,42,50	0.96	2 (4%)	45,47,55	1.25	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	3Y	104	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
69	3PE	1d	206	-	50,50,50	0.91	2 (4%)	53,55,55	0.93	3 (5%)
91	PGV	4A	606	-	50,50,50	0.90	2 (4%)	53,56,56	1.07	3 (5%)
75	CDL	1q	201	-	60,60,99	1.14	5 (8%)	66,72,111	1.39	9 (13%)
69	3PE	3P	506	-	50,50,50	0.89	2 (4%)	53,55,55	1.15	3 (5%)
72	FES	3E	301	49	0,4,4	-	-	-	-	-
69	3PE	1L	703	-	43,43,50	0.98	2 (4%)	46,48,55	1.18	2 (4%)
69	3PE	1L	710	-	37,37,50	1.03	2 (5%)	40,42,55	5.05	5 (12%)
75	CDL	1d	205	-	92,92,99	0.93	4 (4%)	98,104,111	1.19	6 (6%)
69	3PE	1l	202	-	41,41,50	1.02	2 (4%)	44,46,55	1.21	4 (9%)
69	3PE	1g	203	-	32,32,50	1.15	2 (6%)	35,37,55	1.23	3 (8%)
87	PEK	4G	103	-	51,51,52	0.88	2 (3%)	54,56,57	1.11	4 (7%)
69	3PE	3P	519	-	50,50,50	0.87	2 (4%)	53,55,55	1.12	5 (9%)
69	3PE	1d	201	-	47,47,50	0.93	2 (4%)	50,52,55	1.04	2 (4%)
69	3PE	1f	104	-	47,47,50	0.94	2 (4%)	50,52,55	1.05	3 (6%)
70	PC1	3R	303	-	53,53,53	0.97	2 (3%)	59,61,61	1.15	4 (6%)
70	PC1	1B	202	-	45,45,53	6.15	8 (17%)	51,53,61	2.46	12 (23%)
70	PC1	3T	102	-	53,53,53	0.90	3 (5%)	59,61,61	1.07	4 (6%)
69	3PE	1o	201	-	50,50,50	0.89	2 (4%)	53,55,55	1.29	5 (9%)
69	3PE	1Y	212	-	43,43,50	1.00	2 (4%)	46,48,55	1.04	2 (4%)
70	PC1	1B	203	-	47,47,53	0.97	2 (4%)	53,55,61	1.31	6 (11%)
75	CDL	4B	302	-	99,99,99	0.91	4 (4%)	105,111,111	1.05	7 (6%)
72	FES	1G	803	7	0,4,4	-	-	-	-	-
71	SF4	1B	201	2	0,12,12	-	-	-	-	-
85	HEM	3C	501	47	50,50,50	1.59	8 (16%)	67,82,82	1.64	12 (17%)
87	PEK	3X	102	-	52,52,52	0.90	2 (3%)	55,57,57	1.01	5 (9%)
91	PGV	4N	101	-	50,50,50	0.90	2 (4%)	53,56,56	1.10	3 (5%)
91	PGV	4A	609	-	50,50,50	0.90	2 (4%)	53,56,56	1.13	4 (7%)
69	3PE	3A	503	-	50,50,50	0.87	2 (4%)	53,55,55	1.28	4 (7%)
69	3PE	3C	515	-	47,47,50	0.95	2 (4%)	50,52,55	1.11	2 (4%)
75	CDL	1q	202	-	99,99,99	0.90	4 (4%)	105,111,111	1.12	7 (6%)
69	3PE	1e	201	-	50,50,50	0.93	2 (4%)	53,55,55	1.12	4 (7%)
75	CDL	1L	704	-	86,86,99	0.96	5 (5%)	92,98,111	1.28	9 (9%)
69	3PE	3P	505	-	31,31,50	1.17	2 (6%)	34,36,55	1.24	3 (8%)
70	PC1	1d	204	-	38,38,53	1.11	2 (5%)	44,46,61	1.30	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
73	FMN	1F	501	-	33,33,33	0.79	0	48,50,50	0.73	1 (2%)
69	3PE	3G	108	-	32,32,50	1.13	2 (6%)	35,37,55	1.19	2 (5%)
75	CDL	4C	307	-	99,99,99	0.92	4 (4%)	105,111,111	1.03	6 (5%)
69	3PE	3R	305	-	50,50,50	0.91	3 (6%)	53,55,55	1.13	3 (5%)
69	3PE	3P	503	-	50,50,50	0.93	2 (4%)	53,55,55	1.17	4 (7%)
69	3PE	3P	518	-	50,50,50	0.92	2 (4%)	53,55,55	1.11	3 (5%)
69	3PE	3G	101	-	50,50,50	0.89	3 (6%)	53,55,55	1.33	6 (11%)
69	3PE	3P	515	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	3 (5%)
70	PC1	1M	501	-	43,43,53	1.03	2 (4%)	49,51,61	1.19	3 (6%)
92	CUA	4B	301	56	0,1,1	-	-	-	-	-
69	3PE	1b	101	-	41,41,50	0.99	2 (4%)	44,46,55	1.17	4 (9%)
69	3PE	3C	508	-	47,47,50	0.92	2 (4%)	50,52,55	1.13	4 (8%)
69	3PE	3G	105	-	32,32,50	1.12	2 (6%)	35,37,55	1.17	3 (8%)
69	3PE	1B	204	-	50,50,50	0.92	2 (4%)	53,55,55	1.12	4 (7%)
91	PGV	4G	102	-	50,50,50	0.92	2 (4%)	53,56,56	1.01	3 (5%)
69	3PE	3G	104	-	32,32,50	1.16	2 (6%)	35,37,55	1.24	3 (8%)
69	3PE	1B	205	-	50,50,50	0.92	2 (4%)	53,55,55	1.04	3 (5%)
69	3PE	1L	707	-	41,41,50	0.99	3 (7%)	44,46,55	1.26	5 (11%)
69	3PE	1m	204	-	50,50,50	0.91	2 (4%)	53,55,55	1.16	4 (7%)
69	3PE	1Y	210	-	41,41,50	0.98	2 (4%)	44,46,55	1.13	3 (6%)
69	3PE	3C	512	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	4 (7%)
69	3PE	3G	111	-	47,47,50	0.93	2 (4%)	50,52,55	1.07	2 (4%)
71	SF4	1G	802	7	0,12,12	-	-	-	-	-
86	HEC	3Q	501	48	46,50,50	2.58	23 (50%)	58,82,82	2.07	19 (32%)
69	3PE	1k	101	-	45,45,50	0.96	2 (4%)	48,50,55	1.13	4 (8%)
69	3PE	3P	514	-	50,50,50	0.91	2 (4%)	53,55,55	1.02	2 (3%)
69	3PE	3C	517	-	31,31,50	1.13	2 (6%)	34,36,55	1.15	3 (8%)
69	3PE	3C	509	-	50,50,50	0.89	2 (4%)	53,55,55	1.13	4 (7%)
69	3PE	1f	101	-	44,44,50	0.98	2 (4%)	47,49,55	1.02	2 (4%)
69	3PE	3C	504	-	45,45,50	0.29	0	48,50,55	0.34	0
71	SF4	1F	502	6	0,12,12	-	-	-	-	-
69	3PE	1L	701	-	45,45,50	0.96	3 (6%)	48,50,55	1.35	5 (10%)
69	3PE	1L	702	-	44,44,50	0.94	2 (4%)	47,49,55	1.16	5 (10%)
69	3PE	4G	101	-	31,31,50	1.16	2 (6%)	34,36,55	1.18	3 (8%)
72	FES	3R	301	-	0,4,4	-	-	-	-	-
69	3PE	1J	203	-	43,43,50	0.94	3 (6%)	46,48,55	1.19	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
71	SF4	1G	801	7	0,12,12	-	-	-		
75	CDL	3N	502	-	99,99,99	0.88	5 (5%)	105,111,111	1.09	6 (5%)
69	3PE	3Y	103	-	31,31,50	1.15	2 (6%)	34,36,55	1.25	4 (11%)
69	3PE	3Y	105	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	3 (5%)
70	PC1	1h	203	-	45,45,53	1.03	2 (4%)	51,53,61	1.17	4 (7%)
69	3PE	1L	709	-	41,41,50	0.99	2 (4%)	44,46,55	1.28	4 (9%)
69	3PE	3J	104	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	4 (7%)
91	PGV	4C	302	-	50,50,50	0.92	2 (4%)	53,56,56	1.03	3 (5%)
75	CDL	3D	504	-	55,55,99	1.21	6 (10%)	61,67,111	1.35	9 (14%)
91	PGV	4C	305	-	50,50,50	0.90	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	1M	502	-	46,46,50	0.93	2 (4%)	49,51,55	1.07	2 (4%)
69	3PE	3D	503	-	44,44,50	0.96	3 (6%)	47,49,55	1.23	4 (8%)
69	3PE	1Y	209	-	41,41,50	0.96	2 (4%)	44,46,55	1.17	4 (9%)
69	3PE	1m	205	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)
82	PGT	1Y	203	-	50,50,50	0.92	2 (4%)	53,56,56	1.06	3 (5%)
69	3PE	3J	103	-	50,50,50	0.95	2 (4%)	53,55,55	0.99	2 (3%)
69	3PE	3J	105	-	50,50,50	0.91	2 (4%)	53,55,55	1.07	3 (5%)
69	3PE	1L	711	-	40,40,50	1.00	2 (5%)	43,45,55	1.05	2 (4%)
69	3PE	3P	511	-	44,44,50	0.95	2 (4%)	47,49,55	1.14	3 (6%)
69	3PE	3A	502	-	50,50,50	0.92	3 (6%)	53,55,55	1.17	4 (7%)
75	CDL	1d	202	-	85,85,99	0.95	5 (5%)	91,97,111	1.31	10 (10%)
69	3PE	1Y	204	-	30,30,50	1.17	2 (6%)	33,35,55	1.20	3 (9%)
69	3PE	3T	103	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	3G	106	-	32,32,50	1.11	2 (6%)	35,37,55	1.28	4 (11%)
70	PC1	3J	106	-	53,53,53	0.91	2 (3%)	59,61,61	2.70	9 (15%)
70	PC1	1H	402	-	53,53,53	0.92	3 (5%)	59,61,61	1.10	3 (5%)
70	PC1	1A	202	-	34,34,53	1.16	2 (5%)	40,42,61	1.16	4 (10%)
70	PC1	1h	202	-	46,46,53	1.00	2 (4%)	52,54,61	1.13	3 (5%)
91	PGV	4C	301	-	50,50,50	0.90	2 (4%)	53,56,56	1.03	3 (5%)
69	3PE	3Y	107	-	50,50,50	0.91	2 (4%)	53,55,55	1.08	3 (5%)
69	3PE	3P	520	-	50,50,50	0.92	2 (4%)	53,55,55	1.03	3 (5%)
75	CDL	1g	201	-	99,99,99	0.90	4 (4%)	105,111,111	1.03	5 (4%)
70	PC1	3P	509	-	53,53,53	0.90	2 (3%)	59,61,61	1.20	6 (10%)
69	3PE	1h	204	-	46,46,50	0.97	2 (4%)	49,51,55	1.03	2 (4%)
69	3PE	3C	513	-	50,50,50	0.91	2 (4%)	53,55,55	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
69	3PE	3Y	102	-	44,44,50	0.99	2 (4%)	47,49,55	1.04	3 (6%)
70	PC1	1J	202	-	34,34,53	1.15	2 (5%)	40,42,61	1.23	3 (7%)
69	3PE	3Q	504	-	45,45,50	0.98	2 (4%)	48,50,55	1.14	3 (6%)
75	CDL	3P	513	-	99,99,99	0.93	5 (5%)	105,111,111	1.28	11 (10%)
77	GTP	1O	401	78	33,34,34	1.14	2 (6%)	50,54,54	1.77	9 (18%)
75	CDL	3A	501	-	97,97,99	0.91	6 (6%)	103,109,111	1.17	8 (7%)
69	3PE	3J	101	-	46,46,50	0.94	2 (4%)	49,51,55	1.15	2 (4%)
91	PGV	4A	608	-	50,50,50	0.92	2 (4%)	53,56,56	1.02	3 (5%)
85	HEM	3P	501	47	50,50,50	1.59	8 (16%)	67,82,82	1.65	13 (19%)
70	PC1	1H	403	-	47,47,53	0.99	2 (4%)	53,55,61	0.97	3 (5%)
69	3PE	3W	101	-	50,50,50	0.92	2 (4%)	53,55,55	1.02	2 (3%)
69	3PE	3D	502	-	40,40,50	0.31	0	43,45,55	0.40	0
91	PGV	4J	101	-	41,41,50	1.00	2 (4%)	44,47,56	1.11	4 (9%)
69	3PE	1Z	201	-	50,50,50	0.90	2 (4%)	53,55,55	1.14	4 (7%)
69	3PE	1f	103	-	43,43,50	1.01	2 (4%)	45,47,55	1.15	3 (6%)
69	3PE	1g	202	-	50,50,50	0.88	2 (4%)	53,55,55	1.11	5 (9%)
70	PC1	1Y	202	-	34,34,53	1.16	2 (5%)	40,42,61	1.12	3 (7%)
69	3PE	4G	104	-	40,40,50	1.03	2 (5%)	43,45,55	1.15	4 (9%)
69	3PE	3W	103	-	50,50,50	0.93	2 (4%)	53,55,55	3.79	5 (9%)
91	PGV	4C	304	-	50,50,50	0.92	2 (4%)	53,56,56	1.04	4 (7%)
69	3PE	1Y	213	-	50,50,50	0.89	2 (4%)	53,55,55	1.11	3 (5%)
71	SF4	1I	202	9	0,12,12	-	-	-	-	-
69	3PE	3Y	101	-	50,50,50	0.90	2 (4%)	53,55,55	1.04	2 (3%)
75	CDL	1Y	217	-	99,99,99	0.90	4 (4%)	105,111,111	1.03	5 (4%)
69	3PE	3X	105	-	50,50,50	0.92	2 (4%)	53,55,55	0.97	2 (3%)
75	CDL	3Y	106	-	99,99,99	0.90	4 (4%)	105,111,111	1.10	5 (4%)
69	3PE	1A	201	-	46,46,50	0.93	2 (4%)	49,51,55	1.25	5 (10%)
69	3PE	1m	203	-	41,41,50	1.03	2 (4%)	44,46,55	1.13	3 (6%)
69	3PE	3C	505	-	50,50,50	0.90	2 (4%)	53,55,55	1.07	4 (7%)
75	CDL	1N	402	-	76,76,99	1.01	4 (5%)	82,88,111	1.22	7 (8%)
75	CDL	1i	201	-	79,79,99	1.02	5 (6%)	85,91,111	1.31	10 (11%)
69	3PE	1J	201	-	50,50,50	0.92	2 (4%)	53,55,55	1.07	3 (5%)
70	PC1	3X	104	-	53,53,53	0.91	3 (5%)	59,61,61	1.12	5 (8%)
69	3PE	3C	516	-	42,42,50	0.98	2 (4%)	45,47,55	1.13	3 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3P	507	-	-	19/54/54/54	-
69	3PE	3R	304	-	-	18/54/54/54	-
69	3PE	3E	303	-	-	17/52/52/54	-
70	PC1	1Y	207	-	-	11/57/57/57	-
75	CDL	3X	103	-	-	44/110/110/110	-
69	3PE	1L	708	-	-	14/45/45/54	-
69	3PE	3G	107	-	-	8/36/36/54	-
69	3PE	3X	107	-	-	13/54/54/54	-
69	3PE	3C	511	-	-	15/54/54/54	-
75	CDL	1H	401	-	-	20/61/61/110	-
75	CDL	3T	101	-	-	21/67/67/110	-
81	EHZ	1n	201	-	-	5/42/44/45	-
91	PGV	4C	303	-	-	9/55/55/55	-
69	3PE	3W	102	-	-	16/45/45/54	-
69	3PE	3N	501	-	-	15/54/54/54	-
72	FES	1E	301	5	-	-	0/1/1/1
69	3PE	3C	506	-	-	16/50/50/54	-
69	3PE	3J	102	-	-	10/41/41/54	-
69	3PE	3P	508	-	-	16/54/54/54	-
69	3PE	3N	503	-	-	16/54/54/54	-
69	3PE	3P	510	-	-	12/51/51/54	-
75	CDL	4C	306	-	-	39/110/110/110	-
69	3PE	1A	203	-	-	15/44/44/54	-
69	3PE	1Y	211	-	-	9/54/54/54	-
91	PGV	4K	101	-	-	10/47/47/55	-
69	3PE	3G	103	-	-	10/36/36/54	-
69	3PE	1Y	208	-	-	12/54/54/54	-
69	3PE	3Q	502	-	-	8/44/44/54	-
71	SF4	1I	201	9	-	-	0/6/5/5
69	3PE	3E	302	-	-	20/54/54/54	-
70	PC1	1Y	206	-	-	15/49/49/57	-
69	3PE	3X	106	-	-	14/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	1Y	214	-	-	14/54/54/54	-
69	3PE	1Y	216	-	-	14/54/54/54	-
83	AME	1h	201	-	-	2/9/10/12	-
93	PSC	4B	303	-	-	18/55/55/55	-
91	PGV	4A	607	-	-	15/55/55/55	-
69	3PE	3X	101	-	-	16/54/54/54	-
85	HEM	3C	502	-	-	6/14/54/54	-
69	3PE	3C	507	-	-	23/54/54/54	-
69	3PE	1L	712	-	-	20/54/54/54	-
69	3PE	1l	203	-	-	14/36/36/54	-
69	3PE	3C	510	-	-	14/38/38/54	-
69	3PE	3X	108	-	-	14/54/54/54	-
79	NDP	1P	501	-	-	3/34/77/77	0/5/5/5
69	3PE	3P	517	-	-	13/54/54/54	-
69	3PE	1Y	205	-	-	10/43/43/54	-
69	3PE	1Y	201	-	-	12/45/45/54	-
84	MYR	1l	201	-	-	2/12/12/13	-
69	3PE	3S	201	-	-	17/54/54/54	-
85	HEM	3P	502	47	-	8/14/54/54	-
69	3PE	3Q	503	-	-	17/49/49/54	-
76	AYA	1I	203	-	-	2/5/6/8	-
69	3PE	3C	503	-	-	13/54/54/54	-
69	3PE	1L	705	-	-	14/52/52/54	-
75	CDL	3F	201	-	-	38/110/110/110	-
86	HEC	3D	501	48	-	4/13/53/54	-
69	3PE	3P	516	-	-	12/54/54/54	-
69	3PE	3G	102	-	-	13/36/36/54	-
69	3PE	3R	302	-	-	18/54/54/54	-
69	3PE	1N	401	-	-	17/54/54/54	-
69	3PE	3C	514	-	-	8/38/38/54	-
81	EHZ	1T	101	20	-	9/42/44/45	-
69	3PE	1l	204	-	-	19/54/54/54	-
69	3PE	3P	512	-	-	13/51/51/54	-
69	3PE	1L	706	-	-	9/36/36/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
70	PC1	1P	502	-	-	12/36/36/57	-
69	3PE	3G	110	-	-	10/46/46/54	-
69	3PE	1d	203	-	-	27/50/50/54	-
69	3PE	1m	202	-	-	10/45/45/54	-
88	HEA	4A	601	55	-	8/36/76/76	-
69	3PE	3G	109	-	-	15/54/54/54	-
69	3PE	1m	201	-	-	13/53/53/54	-
69	3PE	3P	504	-	-	8/41/41/54	-
69	3PE	1f	102	-	-	13/46/46/54	-
88	HEA	4A	602	55	-	8/36/76/76	-
70	PC1	1H	404	-	-	7/44/44/57	-
69	3PE	1Y	215	-	-	21/46/46/54	-
69	3PE	3Y	104	-	-	20/54/54/54	-
69	3PE	1d	206	-	-	12/54/54/54	-
91	PGV	4A	606	-	-	9/55/55/55	-
75	CDL	1q	201	-	-	15/71/71/110	-
69	3PE	3P	506	-	-	16/54/54/54	-
75	CDL	1d	205	-	-	41/103/103/110	-
69	3PE	1L	703	-	-	13/47/47/54	-
69	3PE	1L	710	-	-	16/41/41/54	-
72	FES	3E	301	49	-	-	0/1/1/1
69	3PE	1l	202	-	-	18/45/45/54	-
69	3PE	1g	203	-	-	13/36/36/54	-
87	PEK	4G	103	-	-	12/55/55/56	-
69	3PE	3P	519	-	-	15/54/54/54	-
69	3PE	1d	201	-	-	33/51/51/54	-
69	3PE	1f	104	-	-	17/51/51/54	-
70	PC1	3R	303	-	-	17/57/57/57	-
70	PC1	1B	202	-	-	20/49/49/57	-
70	PC1	3T	102	-	-	18/57/57/57	-
69	3PE	1o	201	-	-	20/54/54/54	-
69	3PE	1Y	212	-	-	10/47/47/54	-
70	PC1	1B	203	-	-	21/51/51/57	-
75	CDL	4B	302	-	-	27/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
72	FES	1G	803	7	-	-	0/1/1/1
71	SF4	1B	201	2	-	-	0/6/5/5
85	HEM	3C	501	47	-	5/14/54/54	-
87	PEK	3X	102	-	-	19/56/56/56	-
91	PGV	4N	101	-	-	15/55/55/55	-
91	PGV	4A	609	-	-	13/55/55/55	-
69	3PE	3A	503	-	-	18/54/54/54	-
69	3PE	3C	515	-	-	16/51/51/54	-
75	CDL	1q	202	-	-	36/110/110/110	-
69	3PE	1e	201	-	-	13/54/54/54	-
75	CDL	1L	704	-	-	31/97/97/110	-
69	3PE	3P	505	-	-	11/35/35/54	-
70	PC1	1d	204	-	-	24/42/42/57	-
73	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
69	3PE	3G	108	-	-	8/36/36/54	-
75	CDL	4C	307	-	-	19/110/110/110	-
69	3PE	3R	305	-	-	15/54/54/54	-
69	3PE	3P	503	-	-	17/54/54/54	-
69	3PE	3P	518	-	-	16/54/54/54	-
69	3PE	3G	101	-	-	15/54/54/54	-
69	3PE	3P	515	-	-	20/54/54/54	-
70	PC1	1M	501	-	-	18/47/47/57	-
69	3PE	1b	101	-	-	12/45/45/54	-
69	3PE	3C	508	-	-	14/51/51/54	-
69	3PE	3G	105	-	-	15/36/36/54	-
69	3PE	1B	204	-	-	15/54/54/54	-
91	PGV	4G	102	-	-	18/55/55/55	-
69	3PE	3G	104	-	-	14/36/36/54	-
69	3PE	1B	205	-	-	16/54/54/54	-
69	3PE	1L	707	-	-	5/45/45/54	-
69	3PE	1m	204	-	-	13/54/54/54	-
69	3PE	1Y	210	-	-	16/45/45/54	-
69	3PE	3C	512	-	-	16/54/54/54	-
69	3PE	3G	111	-	-	23/51/51/54	-
71	SF4	1G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HEC	3Q	501	48	-	2/14/54/54	-
69	3PE	1k	101	-	-	16/49/49/54	-
69	3PE	3P	514	-	-	15/54/54/54	-
69	3PE	3C	517	-	-	4/35/35/54	-
69	3PE	3C	509	-	-	16/54/54/54	-
69	3PE	1f	101	-	-	20/48/48/54	-
69	3PE	3C	504	-	-	10/49/49/54	-
71	SF4	1F	502	6	-	-	0/6/5/5
69	3PE	1L	701	-	-	16/49/49/54	-
69	3PE	1L	702	-	-	19/48/48/54	-
69	3PE	4G	101	-	-	15/35/35/54	-
72	FES	3R	301	-	-	-	0/1/1/1
69	3PE	1J	203	-	-	6/47/47/54	-
71	SF4	1G	801	7	-	-	0/6/5/5
75	CDL	3N	502	-	-	38/110/110/110	-
69	3PE	3Y	103	-	-	2/35/35/54	-
69	3PE	3Y	105	-	-	5/54/54/54	-
70	PC1	1h	203	-	-	17/49/49/57	-
69	3PE	1L	709	-	-	11/45/45/54	-
69	3PE	3J	104	-	-	14/54/54/54	-
91	PGV	4C	302	-	-	12/55/55/55	-
75	CDL	3D	504	-	-	20/66/66/110	-
91	PGV	4C	305	-	-	11/55/55/55	-
69	3PE	1M	502	-	-	17/50/50/54	-
69	3PE	3D	503	-	-	16/48/48/54	-
69	3PE	1Y	209	-	-	21/45/45/54	-
69	3PE	1m	205	-	-	11/54/54/54	-
82	PGT	1Y	203	-	-	26/55/55/55	-
69	3PE	3J	103	-	-	13/54/54/54	-
69	3PE	3J	105	-	-	12/54/54/54	-
69	3PE	1L	711	-	-	12/44/44/54	-
69	3PE	3P	511	-	-	7/48/48/54	-
69	3PE	3A	502	-	-	16/54/54/54	-
75	CDL	1d	202	-	-	31/96/96/110	-
69	3PE	1Y	204	-	-	5/34/34/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
69	3PE	3T	103	-	-	13/54/54/54	-
69	3PE	3G	106	-	-	11/36/36/54	-
70	PC1	3J	106	-	-	10/57/57/57	-
70	PC1	1H	402	-	-	14/57/57/57	-
70	PC1	1A	202	-	-	10/38/38/57	-
70	PC1	1h	202	-	-	13/50/50/57	-
91	PGV	4C	301	-	-	2/55/55/55	-
69	3PE	3Y	107	-	-	18/54/54/54	-
69	3PE	3P	520	-	-	14/54/54/54	-
75	CDL	1g	201	-	-	46/110/110/110	-
70	PC1	3P	509	-	-	17/57/57/57	-
69	3PE	1h	204	-	-	19/50/50/54	-
69	3PE	3C	513	-	-	14/54/54/54	-
69	3PE	3Y	102	-	-	9/48/48/54	-
70	PC1	1J	202	-	-	17/38/38/57	-
69	3PE	3Q	504	-	-	16/49/49/54	-
75	CDL	3P	513	-	-	15/110/110/110	-
77	GTP	1O	401	78	-	4/22/38/38	0/3/3/3
75	CDL	3A	501	-	-	29/108/108/110	-
69	3PE	3J	101	-	-	19/50/50/54	-
91	PGV	4A	608	-	-	4/55/55/55	-
85	HEM	3P	501	47	-	6/14/54/54	-
70	PC1	1H	403	-	-	12/51/51/57	-
69	3PE	3W	101	-	-	15/54/54/54	-
69	3PE	3D	502	-	-	16/44/44/54	-
91	PGV	4J	101	-	-	12/46/46/55	-
69	3PE	1Z	201	-	-	5/54/54/54	-
69	3PE	1f	103	-	-	10/46/46/54	-
69	3PE	1g	202	-	-	20/54/54/54	-
70	PC1	1Y	202	-	-	19/38/38/57	-
69	3PE	4G	104	-	-	6/44/44/54	-
69	3PE	3W	103	-	-	16/54/54/54	-
91	PGV	4C	304	-	-	6/55/55/55	-
69	3PE	1Y	213	-	-	35/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
71	SF4	1I	202	9	-	-	0/6/5/5
69	3PE	3Y	101	-	-	22/54/54/54	-
75	CDL	1Y	217	-	-	39/110/110/110	-
69	3PE	3X	105	-	-	13/54/54/54	-
75	CDL	3Y	106	-	-	36/110/110/110	-
69	3PE	1A	201	-	-	11/50/50/54	-
69	3PE	1m	203	-	-	15/45/45/54	-
69	3PE	3C	505	-	-	17/54/54/54	-
75	CDL	1N	402	-	-	32/87/87/110	-
75	CDL	1i	201	-	-	12/90/90/110	-
69	3PE	1J	201	-	-	18/54/54/54	-
70	PC1	3X	104	-	-	20/57/57/57	-
69	3PE	3C	516	-	-	8/46/46/54	-

All (584) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1B	202	PC1	C24-C23	40.35	3.52	1.51
88	4A	601	HEA	FE-ND	5.59	2.12	1.94
88	4A	602	HEA	FE-ND	5.55	2.12	1.94
88	4A	601	HEA	FE-NB	5.55	2.12	1.94
88	4A	602	HEA	FE-NB	5.52	2.11	1.94
88	4A	602	HEA	C3B-C2B	5.49	1.47	1.34
85	3C	501	HEM	FE-NB	5.44	2.11	1.94
85	3P	501	HEM	FE-NB	5.42	2.11	1.94
88	4A	601	HEA	C3B-C2B	5.29	1.46	1.34
85	3C	502	HEM	FE-NB	5.23	2.11	1.94
85	3P	502	HEM	FE-NB	5.20	2.10	1.94
86	3Q	501	HEC	C2A-C3A	4.92	1.47	1.36
86	3D	501	HEC	C2A-C3A	4.87	1.47	1.36
88	4A	602	HEA	FE-NC	4.83	2.11	1.95
88	4A	602	HEA	C3D-C2D	4.79	1.47	1.36
88	4A	601	HEA	FE-NC	4.78	2.10	1.95
86	3Q	501	HEC	CHC-C4B	4.77	1.47	1.38
86	3D	501	HEC	CHD-C4C	4.76	1.47	1.38
86	3Q	501	HEC	CHD-C4C	4.76	1.47	1.38
86	3Q	501	HEC	CHA-C1A	4.74	1.47	1.38
86	3D	501	HEC	CHA-C1A	4.70	1.47	1.38
86	3Q	501	HEC	CHB-C4A	4.67	1.47	1.38
88	4A	601	HEA	C3D-C2D	4.59	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	4A	602	HEA	CHC-C4B	4.54	1.47	1.38
86	3D	501	HEC	CHB-C4A	4.54	1.47	1.38
88	4A	601	HEA	C3A-C2A	4.53	1.47	1.37
86	3D	501	HEC	CHC-C4B	4.51	1.47	1.38
69	1f	103	3PE	O31-C31	4.48	1.46	1.33
88	4A	601	HEA	CHC-C4B	4.46	1.47	1.38
69	3Q	503	3PE	O31-C31	4.44	1.46	1.33
85	3C	501	HEM	FE-NC	4.43	2.09	1.95
69	1L	708	3PE	O21-C21	4.42	1.46	1.34
69	3J	103	3PE	O21-C21	4.41	1.46	1.34
88	4A	602	HEA	CHD-C1D	4.40	1.47	1.38
86	3Q	501	HEC	CAC-C3C	4.39	1.49	1.35
69	1l	202	3PE	O21-C21	4.39	1.46	1.34
69	3P	507	3PE	O21-C21	4.38	1.46	1.34
85	3P	501	HEM	FE-NC	4.36	2.09	1.95
69	3C	513	3PE	O31-C31	4.35	1.46	1.33
69	1L	706	3PE	O21-C21	4.35	1.46	1.34
85	3C	502	HEM	FE-NC	4.34	2.09	1.95
75	3P	513	CDL	OA6-CA5	4.34	1.46	1.34
86	3D	501	HEC	CAC-C3C	4.34	1.49	1.35
75	3X	103	CDL	OB6-CB5	4.33	1.46	1.34
69	1J	201	3PE	O31-C31	4.33	1.46	1.33
69	1l	203	3PE	O31-C31	4.32	1.45	1.33
69	3J	103	3PE	O31-C31	4.32	1.45	1.33
69	3Q	504	3PE	O31-C31	4.32	1.45	1.33
75	4C	306	CDL	OB8-CB7	4.32	1.45	1.33
75	4C	307	CDL	OB8-CB7	4.32	1.45	1.33
69	3W	102	3PE	O31-C31	4.31	1.45	1.33
69	3J	101	3PE	O31-C31	4.31	1.45	1.33
69	3C	507	3PE	O31-C31	4.31	1.45	1.33
75	1q	202	CDL	OB8-CB7	4.31	1.45	1.33
88	4A	602	HEA	C1A-NA	4.31	1.47	1.39
69	4G	104	3PE	O31-C31	4.30	1.45	1.33
69	1L	703	3PE	O31-C31	4.30	1.45	1.33
69	1m	203	3PE	O31-C31	4.30	1.45	1.33
69	1e	201	3PE	O31-C31	4.30	1.45	1.33
91	4A	609	PGV	O03-C19	4.30	1.45	1.33
69	1Y	205	3PE	O31-C31	4.30	1.45	1.33
69	3P	503	3PE	O31-C31	4.30	1.45	1.33
75	1g	201	CDL	OA8-CA7	4.30	1.45	1.33
91	4C	304	PGV	O03-C19	4.29	1.45	1.33
69	1Z	201	3PE	O31-C31	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	1B	204	3PE	O31-C31	4.29	1.45	1.33
69	3P	505	3PE	O31-C31	4.29	1.45	1.33
88	4A	601	HEA	CHD-C1D	4.29	1.47	1.38
82	1Y	203	PGT	O3-C11	4.29	1.45	1.33
69	3X	108	3PE	O21-C21	4.28	1.46	1.34
75	1H	401	CDL	OB8-CB7	4.28	1.45	1.33
69	1B	205	3PE	O31-C31	4.28	1.45	1.33
75	4C	306	CDL	OA8-CA7	4.27	1.45	1.33
85	3P	502	HEM	FE-NC	4.27	2.09	1.95
88	4A	602	HEA	CHB-C4A	4.27	1.46	1.38
91	4A	606	PGV	O03-C19	4.27	1.45	1.33
88	4A	602	HEA	C3A-C2A	4.27	1.46	1.37
69	3R	305	3PE	O21-C21	4.27	1.46	1.34
75	4C	307	CDL	OA8-CA7	4.27	1.45	1.33
69	1h	204	3PE	O31-C31	4.26	1.45	1.33
86	3D	501	HEC	CAB-C3B	4.26	1.48	1.35
91	4G	102	PGV	O03-C19	4.26	1.45	1.33
91	4J	101	PGV	O03-C19	4.26	1.45	1.33
69	1d	206	3PE	O31-C31	4.26	1.45	1.33
69	1L	712	3PE	O31-C31	4.26	1.45	1.33
69	1l	204	3PE	O31-C31	4.26	1.45	1.33
93	4B	303	PSC	O03-C19	4.26	1.45	1.33
69	1m	201	3PE	O31-C31	4.26	1.45	1.33
69	3G	107	3PE	O31-C31	4.26	1.45	1.33
69	3Y	105	3PE	O31-C31	4.26	1.45	1.33
69	3Q	502	3PE	O31-C31	4.25	1.45	1.33
69	1L	706	3PE	O31-C31	4.25	1.45	1.33
69	3P	514	3PE	O31-C31	4.25	1.45	1.33
87	3X	102	PEK	O03-C21	4.25	1.45	1.33
69	3Y	102	3PE	O21-C21	4.25	1.46	1.34
69	1h	204	3PE	O21-C21	4.25	1.46	1.34
69	1Y	212	3PE	O31-C31	4.25	1.45	1.33
75	1d	202	CDL	OB6-CB5	4.24	1.46	1.34
69	3G	111	3PE	O31-C31	4.24	1.45	1.33
75	3D	504	CDL	OB8-CB7	4.24	1.45	1.33
69	1f	104	3PE	O31-C31	4.24	1.45	1.33
69	3G	102	3PE	O31-C31	4.24	1.45	1.33
69	3Y	104	3PE	O31-C31	4.24	1.45	1.33
70	1M	501	PC1	O31-C31	4.24	1.45	1.33
69	1Y	205	3PE	O21-C21	4.24	1.46	1.34
69	4G	101	3PE	O31-C31	4.24	1.45	1.33
75	4B	302	CDL	OB8-CB7	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1Y	206	PC1	O31-C31	4.24	1.45	1.33
69	3T	103	3PE	O21-C21	4.24	1.46	1.34
69	3Y	103	3PE	O31-C31	4.23	1.45	1.33
69	1g	203	3PE	O21-C21	4.23	1.46	1.34
91	4C	302	PGV	O03-C19	4.23	1.45	1.33
75	3X	103	CDL	OA8-CA7	4.23	1.45	1.33
69	3G	102	3PE	O21-C21	4.23	1.46	1.34
69	1m	204	3PE	O31-C31	4.22	1.45	1.33
69	3P	517	3PE	O21-C21	4.22	1.46	1.34
75	1d	205	CDL	OA8-CA7	4.22	1.45	1.33
91	4A	608	PGV	O03-C19	4.22	1.45	1.33
69	1A	203	3PE	O31-C31	4.22	1.45	1.33
69	3C	515	3PE	O31-C31	4.22	1.45	1.33
69	1g	202	3PE	O31-C31	4.22	1.45	1.33
69	1f	101	3PE	O21-C21	4.21	1.46	1.34
69	3P	504	3PE	O21-C21	4.21	1.46	1.34
69	1Y	204	3PE	O31-C31	4.21	1.45	1.33
69	1g	203	3PE	O31-C31	4.21	1.45	1.33
70	1Y	202	PC1	O31-C31	4.21	1.45	1.33
69	3X	105	3PE	O31-C31	4.21	1.45	1.33
69	3P	518	3PE	O31-C31	4.21	1.45	1.33
86	3Q	501	HEC	CAB-C3B	4.21	1.48	1.35
75	1L	704	CDL	OA8-CA7	4.20	1.45	1.33
69	3P	503	3PE	O21-C21	4.20	1.46	1.34
91	4C	305	PGV	O03-C19	4.20	1.45	1.33
69	3G	104	3PE	O31-C31	4.20	1.45	1.33
75	1q	201	CDL	OB8-CB7	4.20	1.45	1.33
69	1Y	214	3PE	O31-C31	4.19	1.45	1.33
69	1L	712	3PE	O21-C21	4.19	1.46	1.34
75	1H	401	CDL	OA6-CA5	4.19	1.46	1.34
69	1f	102	3PE	O31-C31	4.19	1.45	1.33
70	1Y	207	PC1	O31-C31	4.19	1.45	1.33
69	3W	103	3PE	O21-C21	4.19	1.46	1.34
69	3C	511	3PE	O31-C31	4.19	1.45	1.33
87	3X	102	PEK	O01-C1	4.19	1.46	1.34
69	3P	515	3PE	O21-C21	4.19	1.46	1.34
69	3W	101	3PE	O21-C21	4.19	1.46	1.34
69	3G	104	3PE	O21-C21	4.18	1.46	1.34
70	1d	204	PC1	O21-C21	4.18	1.46	1.34
70	1H	403	PC1	O31-C31	4.18	1.45	1.33
69	3J	105	3PE	O31-C31	4.18	1.45	1.33
69	3X	106	3PE	O31-C31	4.18	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3W	103	3PE	O31-C31	4.18	1.45	1.33
91	4C	301	PGV	O03-C19	4.18	1.45	1.33
69	1A	201	3PE	O31-C31	4.18	1.45	1.33
75	4B	302	CDL	OA8-CA7	4.18	1.45	1.33
69	1o	201	3PE	O31-C31	4.18	1.45	1.33
69	3G	106	3PE	O31-C31	4.18	1.45	1.33
69	3J	102	3PE	O21-C21	4.18	1.46	1.34
69	3P	510	3PE	O31-C31	4.17	1.45	1.33
69	3X	107	3PE	O31-C31	4.17	1.45	1.33
69	3C	515	3PE	O21-C21	4.17	1.46	1.34
69	3W	101	3PE	O31-C31	4.17	1.45	1.33
75	1H	401	CDL	OA8-CA7	4.17	1.45	1.33
69	3G	105	3PE	O31-C31	4.17	1.45	1.33
91	4K	101	PGV	O03-C19	4.17	1.45	1.33
69	3C	507	3PE	O21-C21	4.17	1.46	1.34
70	1P	502	PC1	O31-C31	4.17	1.45	1.33
69	3X	105	3PE	O21-C21	4.17	1.46	1.34
69	3P	516	3PE	O31-C31	4.16	1.45	1.33
70	1A	202	PC1	O31-C31	4.16	1.45	1.33
75	3Y	106	CDL	OB6-CB5	4.16	1.46	1.34
69	4G	101	3PE	O21-C21	4.16	1.46	1.34
69	3P	520	3PE	O31-C31	4.16	1.45	1.33
69	3Q	504	3PE	O21-C21	4.16	1.46	1.34
69	3X	106	3PE	O21-C21	4.16	1.46	1.34
69	1k	101	3PE	O31-C31	4.15	1.45	1.33
69	3Q	503	3PE	O21-C21	4.15	1.46	1.34
69	3C	512	3PE	O31-C31	4.15	1.45	1.33
69	3Y	107	3PE	O31-C31	4.15	1.45	1.33
69	3P	520	3PE	O21-C21	4.15	1.46	1.34
69	3P	518	3PE	O21-C21	4.15	1.46	1.34
69	1Y	216	3PE	O31-C31	4.15	1.45	1.33
69	1Y	211	3PE	O31-C31	4.14	1.45	1.33
69	3Y	101	3PE	O31-C31	4.14	1.45	1.33
69	1m	203	3PE	O21-C21	4.14	1.46	1.34
75	1N	402	CDL	OB8-CB7	4.14	1.45	1.33
69	3X	101	3PE	O31-C31	4.14	1.45	1.33
69	3P	506	3PE	O31-C31	4.14	1.45	1.33
69	1l	204	3PE	O21-C21	4.14	1.46	1.34
69	1m	205	3PE	O21-C21	4.14	1.46	1.34
69	1L	710	3PE	O31-C31	4.14	1.45	1.33
69	3T	103	3PE	O31-C31	4.14	1.45	1.33
69	3J	104	3PE	O31-C31	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3G	107	3PE	O21-C21	4.14	1.46	1.34
69	3Y	104	3PE	O21-C21	4.14	1.46	1.34
69	3N	503	3PE	O31-C31	4.13	1.45	1.33
69	1d	203	3PE	O31-C31	4.13	1.45	1.33
69	1b	101	3PE	O31-C31	4.13	1.45	1.33
69	3G	108	3PE	O31-C31	4.13	1.45	1.33
70	3T	102	PC1	O31-C31	4.13	1.45	1.33
75	3F	201	CDL	OA8-CA7	4.12	1.45	1.33
91	4A	607	PGV	O03-C19	4.12	1.45	1.33
69	3C	516	3PE	O31-C31	4.12	1.45	1.33
69	1Y	201	3PE	O21-C21	4.12	1.45	1.34
69	1Y	215	3PE	O31-C31	4.12	1.45	1.33
69	3P	512	3PE	O31-C31	4.12	1.45	1.33
69	3C	508	3PE	O21-C21	4.11	1.45	1.34
75	1q	202	CDL	OA8-CA7	4.11	1.45	1.33
69	3Y	102	3PE	O31-C31	4.11	1.45	1.33
88	4A	601	HEA	CHB-C4A	4.11	1.46	1.38
75	3F	201	CDL	OB6-CB5	4.11	1.45	1.34
91	4C	302	PGV	O01-C1	4.11	1.45	1.34
69	3J	105	3PE	O21-C21	4.11	1.45	1.34
75	3F	201	CDL	OA6-CA5	4.11	1.45	1.34
75	3Y	106	CDL	OA8-CA7	4.11	1.45	1.33
91	4A	608	PGV	O01-C1	4.11	1.45	1.34
69	3G	103	3PE	O31-C31	4.11	1.45	1.33
69	1B	205	3PE	O21-C21	4.10	1.45	1.34
88	4A	602	HEA	C4A-NA	4.10	1.47	1.39
69	1Y	210	3PE	O31-C31	4.10	1.45	1.33
69	3C	510	3PE	O31-C31	4.10	1.45	1.33
69	3G	109	3PE	O31-C31	4.10	1.45	1.33
75	1i	201	CDL	OB6-CB5	4.10	1.45	1.34
69	1L	709	3PE	O31-C31	4.10	1.45	1.33
91	4N	101	PGV	O03-C19	4.10	1.45	1.33
69	3G	103	3PE	O21-C21	4.10	1.45	1.34
69	1d	201	3PE	O31-C31	4.10	1.45	1.33
69	3P	504	3PE	O31-C31	4.10	1.45	1.33
69	1Y	208	3PE	O31-C31	4.10	1.45	1.33
91	4C	303	PGV	O01-C1	4.10	1.45	1.34
69	3C	517	3PE	O31-C31	4.10	1.45	1.33
69	1f	103	3PE	O21-C21	4.10	1.45	1.34
69	3C	503	3PE	O21-C21	4.09	1.45	1.34
70	1B	202	PC1	O31-C31	4.09	1.45	1.33
70	3R	303	PC1	O31-C31	4.09	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3P	515	3PE	O31-C31	4.08	1.45	1.33
69	3R	304	3PE	O31-C31	4.08	1.45	1.33
69	1m	202	3PE	O21-C21	4.08	1.45	1.34
91	4A	607	PGV	O01-C1	4.08	1.45	1.34
69	1k	101	3PE	O21-C21	4.08	1.45	1.34
91	4G	102	PGV	O01-C1	4.08	1.45	1.34
88	4A	601	HEA	CHA-C1A	4.08	1.46	1.38
75	4C	307	CDL	OA6-CA5	4.07	1.45	1.34
70	1A	202	PC1	O21-C21	4.07	1.45	1.34
75	1L	704	CDL	OB6-CB5	4.07	1.45	1.34
69	1Y	208	3PE	O21-C21	4.07	1.45	1.34
69	3X	108	3PE	O31-C31	4.07	1.45	1.33
69	3P	514	3PE	O21-C21	4.07	1.45	1.34
69	1M	502	3PE	O31-C31	4.07	1.45	1.33
69	1Y	212	3PE	O21-C21	4.07	1.45	1.34
69	1Y	201	3PE	O31-C31	4.07	1.45	1.33
69	3C	509	3PE	O31-C31	4.07	1.45	1.33
69	3C	505	3PE	O21-C21	4.07	1.45	1.34
75	1Y	217	CDL	OB8-CB7	4.07	1.45	1.33
69	1L	702	3PE	O31-C31	4.07	1.45	1.33
69	3G	108	3PE	O21-C21	4.07	1.45	1.34
69	1Y	209	3PE	O31-C31	4.07	1.45	1.33
69	3C	512	3PE	O21-C21	4.06	1.45	1.34
69	1Y	204	3PE	O21-C21	4.06	1.45	1.34
70	1P	502	PC1	O21-C21	4.06	1.45	1.34
69	3P	505	3PE	O21-C21	4.06	1.45	1.34
91	4K	101	PGV	O01-C1	4.06	1.45	1.34
69	3J	102	3PE	O31-C31	4.06	1.45	1.33
69	1Y	213	3PE	O31-C31	4.06	1.45	1.33
69	3Y	107	3PE	O21-C21	4.06	1.45	1.34
69	3Y	103	3PE	O21-C21	4.05	1.45	1.34
69	1f	101	3PE	O31-C31	4.05	1.45	1.33
69	3J	104	3PE	O21-C21	4.05	1.45	1.34
70	3J	106	PC1	O31-C31	4.05	1.45	1.33
91	4C	303	PGV	O03-C19	4.05	1.45	1.33
69	1Y	216	3PE	O21-C21	4.05	1.45	1.34
70	1Y	202	PC1	O21-C21	4.05	1.45	1.34
70	1H	404	PC1	O21-C21	4.05	1.45	1.34
69	3C	511	3PE	O21-C21	4.05	1.45	1.34
75	4B	302	CDL	OA6-CA5	4.05	1.45	1.34
82	1Y	203	PGT	O2-C31	4.05	1.45	1.34
75	1d	205	CDL	OB6-CB5	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	3Y	106	CDL	OA6-CA5	4.04	1.45	1.34
70	1H	403	PC1	O21-C21	4.04	1.45	1.34
70	3P	509	PC1	O31-C31	4.04	1.45	1.33
69	3C	506	3PE	O31-C31	4.04	1.45	1.33
69	3X	107	3PE	O21-C21	4.04	1.45	1.34
69	1d	203	3PE	O21-C21	4.04	1.45	1.34
69	3C	516	3PE	O21-C21	4.04	1.45	1.34
69	1m	205	3PE	O31-C31	4.03	1.45	1.33
69	3R	304	3PE	O21-C21	4.03	1.45	1.34
69	1J	201	3PE	O21-C21	4.03	1.45	1.34
75	3X	103	CDL	OA6-CA5	4.03	1.45	1.34
75	3F	201	CDL	OB8-CB7	4.03	1.45	1.33
91	4C	301	PGV	O01-C1	4.02	1.45	1.34
70	1J	202	PC1	O31-C31	4.02	1.45	1.33
69	3P	519	3PE	O21-C21	4.02	1.45	1.34
91	4N	101	PGV	O01-C1	4.02	1.45	1.34
75	3T	101	CDL	OB8-CB7	4.02	1.45	1.33
69	3S	201	3PE	O21-C21	4.02	1.45	1.34
75	1Y	217	CDL	OA6-CA5	4.01	1.45	1.34
93	4B	303	PSC	O01-C1	4.01	1.45	1.34
91	4C	304	PGV	O01-C1	4.01	1.45	1.34
69	1b	101	3PE	O21-C21	4.01	1.45	1.34
69	3N	501	3PE	O31-C31	4.01	1.45	1.33
69	3Y	101	3PE	O21-C21	4.01	1.45	1.34
69	3Y	105	3PE	O21-C21	4.01	1.45	1.34
69	3P	511	3PE	O21-C21	4.01	1.45	1.34
69	3P	511	3PE	O31-C31	4.01	1.45	1.33
69	1Y	214	3PE	O21-C21	4.01	1.45	1.34
69	1l	202	3PE	O31-C31	4.00	1.45	1.33
69	1L	705	3PE	O31-C31	4.00	1.45	1.33
69	1m	201	3PE	O21-C21	4.00	1.45	1.34
69	1Y	211	3PE	O21-C21	4.00	1.45	1.34
70	1Y	207	PC1	O21-C21	4.00	1.45	1.34
87	4G	103	PEK	O03-C21	4.00	1.45	1.33
88	4A	601	HEA	C1A-NA	4.00	1.47	1.39
75	4B	302	CDL	OB6-CB5	4.00	1.45	1.34
91	4C	305	PGV	O01-C1	3.99	1.45	1.34
69	3S	201	3PE	O31-C31	3.99	1.45	1.33
75	1q	202	CDL	OB6-CB5	3.99	1.45	1.34
69	3G	110	3PE	O31-C31	3.99	1.45	1.33
70	1h	202	PC1	O21-C21	3.99	1.45	1.34
69	3J	101	3PE	O21-C21	3.99	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	4A	601	HEA	C4A-NA	3.98	1.47	1.39
69	3C	505	3PE	O31-C31	3.98	1.45	1.33
87	4G	103	PEK	O01-C1	3.98	1.45	1.34
69	3P	516	3PE	O21-C21	3.98	1.45	1.34
69	3G	111	3PE	O21-C21	3.98	1.45	1.34
75	1i	201	CDL	OA8-CA7	3.98	1.45	1.33
75	1g	201	CDL	OB6-CB5	3.98	1.45	1.34
69	4G	104	3PE	O21-C21	3.98	1.45	1.34
69	1d	206	3PE	O21-C21	3.98	1.45	1.34
75	1g	201	CDL	OB8-CB7	3.98	1.44	1.33
69	1A	203	3PE	O21-C21	3.98	1.45	1.34
69	3G	110	3PE	O21-C21	3.97	1.45	1.34
70	1J	202	PC1	O21-C21	3.97	1.45	1.34
69	3X	101	3PE	O21-C21	3.97	1.45	1.34
69	3P	517	3PE	O31-C31	3.97	1.44	1.33
75	1g	201	CDL	OA6-CA5	3.97	1.45	1.34
91	4J	101	PGV	O01-C1	3.97	1.45	1.34
75	3P	513	CDL	OB8-CB7	3.97	1.44	1.33
69	3C	514	3PE	O31-C31	3.97	1.44	1.33
69	3Q	502	3PE	O21-C21	3.97	1.45	1.34
75	4C	307	CDL	OB6-CB5	3.96	1.45	1.34
91	4A	606	PGV	O01-C1	3.96	1.45	1.34
75	3Y	106	CDL	OB8-CB7	3.96	1.44	1.33
75	4C	306	CDL	OB6-CB5	3.96	1.45	1.34
70	1Y	206	PC1	O21-C21	3.96	1.45	1.34
69	3C	508	3PE	O31-C31	3.96	1.44	1.33
75	1i	201	CDL	OA6-CA5	3.96	1.45	1.34
69	1f	102	3PE	O21-C21	3.96	1.45	1.34
69	3C	517	3PE	O21-C21	3.95	1.45	1.34
70	1h	202	PC1	O31-C31	3.95	1.44	1.33
69	1M	502	3PE	O21-C21	3.95	1.45	1.34
69	1e	201	3PE	O21-C21	3.95	1.45	1.34
70	1H	404	PC1	O31-C31	3.95	1.44	1.33
75	4C	306	CDL	OA6-CA5	3.95	1.45	1.34
70	1H	402	PC1	O21-C21	3.95	1.45	1.34
75	3A	501	CDL	OB6-CB5	3.94	1.45	1.34
69	1m	204	3PE	O21-C21	3.94	1.45	1.34
69	1N	401	3PE	O21-C21	3.93	1.45	1.34
70	3R	303	PC1	O21-C21	3.93	1.45	1.34
69	1m	202	3PE	O31-C31	3.93	1.44	1.33
69	1L	709	3PE	O21-C21	3.93	1.45	1.34
70	1h	203	PC1	O21-C21	3.92	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
75	3N	502	CDL	OA8-CA7	3.92	1.44	1.33
69	3D	503	3PE	O21-C21	3.92	1.45	1.34
70	3J	106	PC1	O21-C21	3.92	1.45	1.34
75	1H	401	CDL	OB6-CB5	3.92	1.45	1.34
69	3C	503	3PE	O31-C31	3.91	1.44	1.33
70	1h	203	PC1	O31-C31	3.91	1.44	1.33
75	1N	402	CDL	OA6-CA5	3.91	1.45	1.34
69	1L	711	3PE	O31-C31	3.91	1.44	1.33
69	3A	502	3PE	O31-C31	3.91	1.44	1.33
69	1J	203	3PE	O31-C31	3.91	1.44	1.33
75	1N	402	CDL	OA8-CA7	3.91	1.44	1.33
69	3C	506	3PE	O21-C21	3.91	1.45	1.34
69	3G	105	3PE	O21-C21	3.91	1.45	1.34
75	1Y	217	CDL	OA8-CA7	3.91	1.44	1.33
70	1B	202	PC1	O21-C21	3.90	1.45	1.34
75	1N	402	CDL	OB6-CB5	3.90	1.45	1.34
69	3E	302	3PE	O21-C21	3.90	1.45	1.34
69	1f	104	3PE	O21-C21	3.89	1.45	1.34
69	1B	204	3PE	O21-C21	3.89	1.45	1.34
75	3T	101	CDL	OA6-CA5	3.88	1.45	1.34
69	1l	203	3PE	O21-C21	3.88	1.45	1.34
70	1B	203	PC1	O21-C21	3.88	1.45	1.34
69	1L	711	3PE	O21-C21	3.88	1.45	1.34
69	3P	512	3PE	O21-C21	3.88	1.45	1.34
69	3D	503	3PE	O31-C31	3.88	1.44	1.33
69	3W	102	3PE	O21-C21	3.88	1.45	1.34
69	1L	708	3PE	O31-C31	3.88	1.44	1.33
69	3A	503	3PE	O31-C31	3.87	1.44	1.33
69	3G	101	3PE	O31-C31	3.87	1.44	1.33
75	3P	513	CDL	OA8-CA7	3.87	1.44	1.33
69	3G	109	3PE	O21-C21	3.87	1.45	1.34
75	3D	504	CDL	OA6-CA5	3.87	1.45	1.34
75	1Y	217	CDL	OB6-CB5	3.87	1.45	1.34
75	1d	205	CDL	OB8-CB7	3.86	1.44	1.33
69	3G	106	3PE	O21-C21	3.86	1.45	1.34
69	1L	703	3PE	O21-C21	3.86	1.45	1.34
69	1L	705	3PE	O21-C21	3.86	1.45	1.34
69	1d	201	3PE	O21-C21	3.86	1.45	1.34
69	3A	502	3PE	O21-C21	3.86	1.45	1.34
69	1Y	213	3PE	O21-C21	3.85	1.45	1.34
75	1d	202	CDL	OA8-CA7	3.85	1.44	1.33
69	3C	509	3PE	O21-C21	3.85	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	4A	609	PGV	O01-C1	3.85	1.45	1.34
69	3E	302	3PE	O31-C31	3.84	1.44	1.33
75	3X	103	CDL	OB8-CB7	3.83	1.44	1.33
69	3C	513	3PE	O21-C21	3.83	1.45	1.34
75	3A	501	CDL	OB8-CB7	3.83	1.44	1.33
69	1o	201	3PE	O21-C21	3.83	1.45	1.34
70	1H	402	PC1	O31-C31	3.83	1.44	1.33
75	3A	501	CDL	OA8-CA7	3.82	1.44	1.33
69	3P	506	3PE	O21-C21	3.82	1.45	1.34
75	1d	205	CDL	OA6-CA5	3.82	1.45	1.34
70	1d	204	PC1	O31-C31	3.82	1.44	1.33
69	3P	519	3PE	O31-C31	3.82	1.44	1.33
69	3N	503	3PE	O21-C21	3.82	1.45	1.34
69	1L	710	3PE	O21-C21	3.81	1.45	1.34
69	1L	701	3PE	O21-C21	3.80	1.45	1.34
69	3P	510	3PE	O21-C21	3.80	1.45	1.34
75	1q	201	CDL	OB6-CB5	3.80	1.45	1.34
75	3D	504	CDL	OA8-CA7	3.79	1.44	1.33
75	1q	201	CDL	OA8-CA7	3.78	1.44	1.33
69	1Y	210	3PE	O21-C21	3.78	1.45	1.34
86	3Q	501	HEC	CHD-C1D	3.78	1.47	1.39
86	3D	501	HEC	CHD-C1D	3.77	1.47	1.39
69	1N	401	3PE	O31-C31	3.76	1.44	1.33
69	1L	702	3PE	O21-C21	3.76	1.44	1.34
75	3N	502	CDL	OB8-CB7	3.75	1.44	1.33
75	1q	202	CDL	OA6-CA5	3.75	1.44	1.34
88	4A	602	HEA	CHA-C1A	3.75	1.45	1.38
69	3R	302	3PE	O21-C21	3.75	1.44	1.34
86	3Q	501	HEC	CHC-C1C	3.74	1.47	1.39
86	3D	501	HEC	CHA-C4D	3.74	1.47	1.39
69	3G	101	3PE	O21-C21	3.74	1.44	1.34
69	1A	201	3PE	O21-C21	3.73	1.44	1.34
69	1L	707	3PE	O31-C31	3.72	1.44	1.33
70	1M	501	PC1	O21-C21	3.72	1.44	1.34
69	3E	303	3PE	O31-C31	3.70	1.44	1.33
70	1B	203	PC1	O31-C31	3.70	1.44	1.33
69	1Z	201	3PE	O21-C21	3.70	1.44	1.34
69	1J	203	3PE	O21-C21	3.70	1.44	1.34
69	1Y	209	3PE	O21-C21	3.69	1.44	1.34
75	1q	201	CDL	OA6-CA5	3.69	1.44	1.34
75	1L	704	CDL	OB8-CB7	3.69	1.44	1.33
69	3P	507	3PE	O31-C31	3.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	3P	508	3PE	O31-C31	3.67	1.44	1.33
86	3D	501	HEC	CHC-C1C	3.67	1.47	1.39
75	1i	201	CDL	OB8-CB7	3.65	1.44	1.33
86	3Q	501	HEC	CHB-C1B	3.65	1.47	1.39
69	3C	514	3PE	O21-C21	3.65	1.44	1.34
75	1L	704	CDL	OA6-CA5	3.64	1.44	1.34
75	3A	501	CDL	OA6-CA5	3.63	1.44	1.34
69	1L	707	3PE	O21-C21	3.63	1.44	1.34
69	1g	202	3PE	O21-C21	3.63	1.44	1.34
69	1Y	215	3PE	O21-C21	3.63	1.44	1.34
70	3P	509	PC1	O21-C21	3.62	1.44	1.34
70	3X	104	PC1	O21-C21	3.61	1.44	1.34
86	3Q	501	HEC	CHA-C4D	3.60	1.47	1.39
75	3T	101	CDL	OA8-CA7	3.60	1.43	1.33
75	1d	202	CDL	OA6-CA5	3.59	1.44	1.34
69	3A	503	3PE	O21-C21	3.59	1.44	1.34
69	3R	305	3PE	O31-C31	3.58	1.43	1.33
69	1L	701	3PE	O31-C31	3.57	1.43	1.33
70	3T	102	PC1	O21-C21	3.56	1.44	1.34
88	4A	602	HEA	CHD-C4C	3.56	1.47	1.39
75	3N	502	CDL	OB6-CB5	3.56	1.44	1.34
69	3N	501	3PE	O21-C21	3.55	1.44	1.34
69	3E	303	3PE	O21-C21	3.54	1.44	1.34
75	3N	502	CDL	OA6-CA5	3.54	1.44	1.34
75	3P	513	CDL	OB6-CB5	3.52	1.44	1.34
88	4A	601	HEA	CHC-C1C	3.48	1.47	1.39
69	3R	302	3PE	O31-C31	3.48	1.43	1.33
75	3T	101	CDL	OB6-CB5	3.47	1.44	1.34
88	4A	602	HEA	CHC-C1C	3.47	1.47	1.39
75	3D	504	CDL	OB6-CB5	3.46	1.44	1.34
70	3X	104	PC1	O31-C31	3.45	1.43	1.33
88	4A	601	HEA	CHD-C4C	3.43	1.47	1.39
85	3P	502	HEM	C1B-NB	-3.43	1.34	1.40
75	1d	202	CDL	OB8-CB7	3.43	1.43	1.33
88	4A	602	HEA	CHB-C1B	3.43	1.47	1.39
85	3C	502	HEM	C1B-NB	-3.42	1.34	1.40
69	3C	510	3PE	O21-C2	-3.41	1.38	1.46
86	3D	501	HEC	CHB-C1B	3.40	1.47	1.39
85	3C	501	HEM	C1B-NB	-3.38	1.34	1.40
85	3P	501	HEM	C1B-NB	-3.34	1.34	1.40
85	3P	502	HEM	C4D-ND	-3.34	1.34	1.40
69	3P	508	3PE	O21-C21	3.30	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	4A	601	HEA	CHA-C4D	3.28	1.46	1.39
85	3C	502	HEM	C4D-ND	-3.25	1.34	1.40
69	3C	510	3PE	O21-C21	3.24	1.43	1.34
86	3D	501	HEC	C3D-C2D	3.23	1.47	1.38
86	3Q	501	HEC	C3D-C2D	3.20	1.47	1.38
85	3P	501	HEM	C4D-ND	-3.20	1.34	1.40
88	4A	602	HEA	CHA-C4D	3.14	1.46	1.39
88	4A	601	HEA	CHB-C1B	3.10	1.46	1.39
85	3C	501	HEM	C4D-ND	-3.07	1.34	1.40
77	1O	401	GTP	C5-C4	2.93	1.46	1.38
88	4A	601	HEA	C4B-C3B	2.84	1.49	1.44
88	4A	602	HEA	C1D-ND	-2.76	1.35	1.40
86	3Q	501	HEC	C1A-NA	-2.75	1.34	1.39
88	4A	601	HEA	C1D-ND	-2.69	1.35	1.40
70	1B	202	PC1	C25-C24	-2.66	1.38	1.51
86	3Q	501	HEC	C4D-ND	-2.64	1.34	1.39
69	1L	701	3PE	O21-C2	-2.63	1.40	1.46
85	3C	501	HEM	C1C-C2C	-2.63	1.40	1.45
88	4A	602	HEA	C4B-NB	-2.61	1.35	1.40
86	3D	501	HEC	C4D-ND	-2.56	1.34	1.39
85	3P	502	HEM	C1C-C2C	-2.56	1.40	1.45
88	4A	602	HEA	C1C-C2C	2.52	1.49	1.43
88	4A	601	HEA	C4B-NB	-2.52	1.35	1.40
88	4A	602	HEA	C4B-C3B	2.51	1.49	1.44
85	3C	502	HEM	C1C-C2C	-2.51	1.40	1.45
88	4A	601	HEA	C1C-C2C	2.51	1.49	1.43
86	3D	501	HEC	C1A-NA	-2.50	1.34	1.39
77	1O	401	GTP	C6-N1	-2.47	1.34	1.38
86	3Q	501	HEC	C1B-C2B	2.46	1.48	1.43
86	3D	501	HEC	C4B-NB	-2.46	1.35	1.39
86	3Q	501	HEC	C1C-C2C	2.45	1.48	1.43
86	3Q	501	HEC	C4B-NB	-2.43	1.35	1.39
85	3P	502	HEM	FE-ND	-2.42	1.87	1.94
86	3Q	501	HEC	C1D-C2D	2.41	1.48	1.43
88	4A	601	HEA	C4D-C3D	2.41	1.49	1.45
86	3D	501	HEC	C4A-NA	-2.40	1.35	1.39
86	3D	501	HEC	C1B-C2B	2.38	1.48	1.43
70	3X	104	PC1	O21-C2	-2.38	1.41	1.46
69	1L	707	3PE	O21-C2	-2.37	1.41	1.46
75	3P	513	CDL	OB6-CB4	-2.36	1.41	1.46
86	3D	501	HEC	C1D-C2D	2.36	1.48	1.43
75	3D	504	CDL	OB6-CB4	-2.36	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	3Q	501	HEC	C4C-NC	-2.35	1.35	1.39
69	3E	303	3PE	O21-C2	-2.34	1.41	1.46
69	3N	501	3PE	O21-C2	-2.34	1.41	1.46
86	3D	501	HEC	C1C-C2C	2.32	1.48	1.43
86	3Q	501	HEC	C4A-NA	-2.31	1.35	1.39
85	3P	501	HEM	C1C-C2C	-2.31	1.40	1.45
86	3D	501	HEC	C4C-NC	-2.30	1.35	1.39
88	4A	602	HEA	C4C-NC	-2.28	1.35	1.39
86	3Q	501	HEC	C1D-ND	-2.27	1.35	1.39
85	3C	502	HEM	C1D-ND	-2.27	1.34	1.38
85	3P	502	HEM	C1D-ND	-2.26	1.34	1.38
88	4A	601	HEA	C4C-NC	-2.26	1.35	1.39
75	1d	202	CDL	OA6-CA4	-2.25	1.41	1.46
86	3D	501	HEC	C1D-ND	-2.24	1.35	1.39
69	3P	508	3PE	O21-C2	-2.24	1.41	1.46
69	3R	305	3PE	O21-C2	-2.24	1.41	1.46
85	3C	501	HEM	C4B-NB	-2.22	1.34	1.38
69	3A	502	3PE	O21-C2	-2.22	1.41	1.46
75	3T	101	CDL	OA6-CA4	-2.22	1.41	1.46
85	3C	502	HEM	C3C-C4C	-2.22	1.42	1.46
88	4A	602	HEA	C1D-C2D	2.21	1.49	1.44
70	1B	202	PC1	C2B-C2A	-2.20	1.34	1.50
85	3P	502	HEM	C3C-C4C	-2.20	1.42	1.46
85	3C	502	HEM	C4B-NB	-2.19	1.34	1.38
85	3C	501	HEM	FE-ND	-2.18	1.88	1.94
86	3Q	501	HEC	C1B-NB	-2.18	1.35	1.39
85	3P	501	HEM	FE-ND	-2.17	1.88	1.94
88	4A	601	HEA	C11-C3B	-2.17	1.48	1.51
70	1H	404	PC1	C12-N	-2.16	1.44	1.51
75	3T	101	CDL	OB6-CB4	-2.16	1.41	1.46
75	3A	501	CDL	OB6-CB4	-2.16	1.41	1.46
69	3R	302	3PE	O21-C2	-2.16	1.41	1.46
69	3G	101	3PE	O21-C2	-2.15	1.41	1.46
75	3D	504	CDL	OA6-CA4	-2.14	1.41	1.46
70	3T	102	PC1	O21-C2	-2.14	1.41	1.46
75	1L	704	CDL	OA6-CA4	-2.14	1.41	1.46
85	3P	501	HEM	C1D-ND	-2.13	1.34	1.38
86	3Q	501	HEC	C1C-NC	-2.13	1.35	1.39
85	3P	502	HEM	C4B-NB	-2.13	1.34	1.38
69	3P	508	3PE	O31-C3	-2.13	1.40	1.45
75	3A	501	CDL	OA6-CA4	-2.12	1.41	1.46
85	3P	501	HEM	C3C-C4C	-2.11	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
70	1B	202	PC1	C26-C25	-2.11	1.41	1.51
75	1q	201	CDL	OA6-CA4	-2.11	1.41	1.46
69	1J	203	3PE	O21-C2	-2.10	1.41	1.46
70	1B	202	PC1	C29-C28	-2.10	1.41	1.51
86	3D	501	HEC	C1B-NB	-2.09	1.35	1.39
85	3C	502	HEM	FE-ND	-2.09	1.88	1.94
70	1B	202	PC1	C27-C26	-2.08	1.41	1.51
69	3N	503	3PE	O21-C2	-2.07	1.41	1.46
75	3N	502	CDL	OB6-CB4	-2.06	1.41	1.46
69	3D	503	3PE	O21-C2	-2.05	1.41	1.46
75	1i	201	CDL	OB6-CB4	-2.04	1.41	1.46
86	3D	501	HEC	C1C-NC	-2.04	1.35	1.39
70	1H	402	PC1	O21-C2	-2.04	1.41	1.46
86	3D	501	HEC	C4D-C3D	2.02	1.48	1.44
85	3C	501	HEM	C1D-ND	-2.00	1.34	1.38

All (916) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1L	710	3PE	O21-C21-C22	22.31	159.74	111.48
69	3Q	502	3PE	O21-C21-C22	21.62	158.26	111.48
69	3Q	502	3PE	O21-C21-O22	-19.37	78.41	123.70
69	3W	103	3PE	O31-C31-O32	-19.03	76.02	123.63
69	1L	710	3PE	O21-C21-O22	-18.92	79.47	123.70
69	3W	103	3PE	O31-C31-C32	15.48	159.05	111.83
70	3J	106	PC1	C15-N-C14	-11.85	77.84	108.98
70	3J	106	PC1	C15-N-C13	-11.65	78.38	108.98
69	3Q	502	3PE	O22-C21-C22	-11.23	79.85	123.78
69	1L	710	3PE	O22-C21-C22	-11.12	80.30	123.78
69	3W	103	3PE	O32-C31-C32	-10.41	83.06	123.78
70	1B	202	PC1	C2B-C2A-C29	-9.95	46.16	113.36
70	3J	106	PC1	C15-N-C12	-8.28	77.01	109.91
69	3C	510	3PE	C2-O21-C21	-6.90	101.29	117.80
88	4A	602	HEA	C3D-C4D-ND	6.73	116.86	110.35
88	4A	601	HEA	C3D-C4D-ND	6.41	116.55	110.35
81	1T	101	EHZ	C10-S1-C9	6.10	119.88	101.84
81	1n	201	EHZ	C10-S1-C9	6.03	119.68	101.84
88	4A	601	HEA	C2B-C1B-NB	6.02	116.86	109.90
77	1O	401	GTP	C5-C4-N3	-5.93	118.94	128.39
70	1B	202	PC1	C25-C24-C23	5.77	143.51	114.37
88	4A	602	HEA	C2D-C1D-ND	5.65	116.33	109.84
69	3A	503	3PE	C2-O21-C21	-5.64	104.29	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	3P	501	HEM	CHC-C4B-NB	5.64	130.49	124.42
70	1B	202	PC1	C28-C27-C26	-5.53	86.39	114.37
85	3C	501	HEM	CHC-C4B-NB	5.53	130.37	124.42
88	4A	601	HEA	C2D-C1D-ND	5.51	116.17	109.84
88	4A	602	HEA	C3B-C4B-NB	5.50	116.16	109.84
88	4A	602	HEA	C2A-C1A-NA	5.50	115.63	110.32
88	4A	601	HEA	C3C-C2C-C1C	-5.50	100.69	107.17
88	4A	602	HEA	C3C-C2C-C1C	-5.48	100.71	107.17
88	4A	602	HEA	C2B-C1B-NB	5.47	116.22	109.90
75	1L	704	CDL	OB6-CB5-C51	5.44	123.26	111.48
88	4A	601	HEA	C3C-C4C-NC	5.43	114.37	109.80
70	1B	202	PC1	C26-C25-C24	-5.42	86.98	114.37
88	4A	601	HEA	C3B-C4B-NB	5.39	116.03	109.84
69	1o	201	3PE	O21-C21-C22	5.36	123.08	111.48
75	1i	201	CDL	OB6-CB5-C51	5.36	123.07	111.48
88	4A	602	HEA	C3C-C4C-NC	5.15	114.14	109.80
77	1O	401	GTP	C2-N3-C4	5.14	121.15	112.30
75	1d	202	CDL	OB6-CB5-C51	5.12	122.55	111.48
75	3P	513	CDL	OB6-CB5-C51	5.11	122.53	111.48
70	1B	202	PC1	O21-C21-C22	5.06	122.44	111.48
86	3D	501	HEC	C2A-C1A-NA	5.01	115.15	110.32
70	1B	203	PC1	O21-C21-C22	5.00	122.30	111.48
88	4A	601	HEA	C2A-C1A-NA	4.98	115.13	110.32
86	3Q	501	HEC	C2A-C1A-NA	4.92	115.07	110.32
69	3G	104	3PE	O21-C21-C22	4.90	122.08	111.48
69	3P	503	3PE	O21-C21-C22	4.88	122.05	111.48
79	1P	501	NDP	P2B-O2B-C2B	-4.88	110.40	123.43
85	3P	502	HEM	CHC-C4B-NB	4.86	129.66	124.42
70	3R	303	PC1	O21-C21-C22	4.83	121.93	111.48
70	1B	202	PC1	C27-C26-C25	-4.80	90.10	114.37
70	1d	204	PC1	O21-C21-C22	4.75	121.75	111.48
85	3C	502	HEM	CHC-C4B-NB	4.74	129.53	124.42
75	3Y	106	CDL	OB6-CB5-C51	4.72	121.70	111.48
75	1d	205	CDL	OA6-CA5-C11	4.67	121.59	111.48
70	1h	203	PC1	O21-C21-C22	4.67	121.59	111.48
75	1q	202	CDL	OA6-CA5-C11	4.66	121.56	111.48
69	3R	305	3PE	O21-C21-C22	4.64	121.53	111.48
69	1L	708	3PE	O21-C21-C22	4.64	121.52	111.48
69	3G	101	3PE	O21-C21-C22	4.63	121.51	111.48
69	3J	102	3PE	O21-C21-C22	4.63	121.50	111.48
69	1m	204	3PE	O21-C21-C22	4.62	121.47	111.48
75	1q	201	CDL	OB6-CB5-C51	4.60	121.44	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1d	203	3PE	O21-C21-C22	4.60	121.42	111.48
75	3D	504	CDL	OA6-CA5-C11	4.59	121.40	111.48
85	3P	501	HEM	CHD-C1D-ND	4.58	129.35	124.42
69	1B	204	3PE	O21-C21-C22	4.58	121.38	111.48
86	3D	501	HEC	C3D-C4D-ND	4.56	115.21	110.15
69	3J	105	3PE	O21-C21-C22	4.55	121.33	111.48
75	1i	201	CDL	OA6-CA5-C11	4.55	121.32	111.48
70	3P	509	PC1	O21-C21-C22	4.54	121.30	111.48
69	1g	203	3PE	O21-C21-C22	4.54	121.29	111.48
86	3Q	501	HEC	C3D-C4D-ND	4.53	115.18	110.15
69	3C	508	3PE	O21-C21-C22	4.52	121.26	111.48
77	1O	401	GTP	N9-C4-N3	4.51	134.97	125.95
69	3C	509	3PE	O21-C21-C22	4.49	121.20	111.48
70	1M	501	PC1	O21-C21-C22	4.49	121.19	111.48
69	1N	401	3PE	O21-C21-C22	4.48	121.17	111.48
75	1q	201	CDL	OA6-CA5-C11	4.46	121.13	111.48
69	3G	103	3PE	O21-C21-C22	4.46	121.13	111.48
75	3P	513	CDL	CB4-OB6-CB5	-4.46	107.12	117.80
85	3C	501	HEM	CHD-C1D-ND	4.43	129.19	124.42
69	1e	201	3PE	O21-C21-C22	4.41	121.02	111.48
88	4A	602	HEA	C1D-C2D-C3D	-4.41	102.34	106.98
75	3P	513	CDL	OA6-CA5-C11	4.41	121.02	111.48
69	1A	203	3PE	O21-C21-C22	4.39	120.98	111.48
69	1L	703	3PE	O21-C21-C22	4.39	120.97	111.48
75	3A	501	CDL	OA6-CA5-C11	4.38	120.96	111.48
75	3T	101	CDL	OA6-CA5-C11	4.38	120.96	111.48
69	4G	101	3PE	O21-C21-C22	4.38	120.95	111.48
70	3J	106	PC1	O21-C21-C22	4.35	120.90	111.48
69	3C	515	3PE	O21-C21-C22	4.35	120.89	111.48
69	1L	712	3PE	O21-C21-C22	4.34	120.88	111.48
75	3F	201	CDL	OA6-CA5-C11	4.33	120.85	111.48
69	1k	101	3PE	O21-C21-C22	4.33	120.84	111.48
69	3P	511	3PE	O21-C21-C22	4.32	120.83	111.48
75	3X	103	CDL	OA6-CA5-C11	4.32	120.82	111.48
69	1L	707	3PE	O21-C21-C22	4.30	120.78	111.48
69	3P	508	3PE	O21-C21-C22	4.30	120.78	111.48
69	3W	103	3PE	O21-C21-C22	4.29	120.75	111.48
69	1l	202	3PE	O21-C21-C22	4.27	120.73	111.48
69	1Y	216	3PE	O21-C21-C22	4.27	120.71	111.48
69	3Y	107	3PE	O21-C21-C22	4.26	120.70	111.48
69	1L	701	3PE	O21-C21-C22	4.26	120.70	111.48
69	1A	201	3PE	O21-C21-C22	4.26	120.70	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	3E	303	3PE	O21-C21-C22	4.26	120.69	111.48
69	1L	709	3PE	O21-C21-C22	4.25	120.68	111.48
88	4A	602	HEA	C3A-C2A-C1A	-4.25	103.03	107.05
75	1d	205	CDL	CA4-OA6-CA5	-4.25	107.64	117.80
75	1N	402	CDL	OB6-CB5-C51	4.24	120.65	111.48
69	3P	515	3PE	O21-C21-C22	4.23	120.64	111.48
69	3C	512	3PE	O21-C21-C22	4.23	120.64	111.48
75	4B	302	CDL	OB6-CB5-C51	4.23	120.64	111.48
69	3Q	503	3PE	O21-C21-C22	4.23	120.63	111.48
70	1H	402	PC1	O21-C21-C22	4.21	120.60	111.48
69	3R	302	3PE	O21-C21-C22	4.21	120.59	111.48
75	3F	201	CDL	OB6-CB5-C51	4.21	120.59	111.48
70	1Y	207	PC1	O21-C21-C22	4.20	120.56	111.48
69	3C	516	3PE	O21-C21-C22	4.19	120.55	111.48
70	1J	202	PC1	O21-C21-C22	4.19	120.55	111.48
75	3A	501	CDL	OB6-CB5-C51	4.19	120.54	111.48
91	4N	101	PGV	O01-C1-C2	4.19	120.54	111.48
87	4G	103	PEK	O01-C1-C2	4.18	120.52	111.48
85	3C	502	HEM	CHD-C1D-ND	4.17	128.91	124.42
69	1m	202	3PE	O21-C21-C22	4.16	120.48	111.48
69	3J	101	3PE	O21-C21-C22	4.16	120.47	111.48
69	3E	302	3PE	O21-C21-C22	4.15	120.45	111.48
69	3P	504	3PE	O21-C21-C22	4.14	120.45	111.48
69	3C	510	3PE	O21-C21-C22	4.14	120.44	111.48
91	4C	304	PGV	O01-C1-C2	4.14	120.44	111.48
69	3C	505	3PE	O21-C21-C22	4.14	120.43	111.48
69	3D	503	3PE	O21-C21-C22	4.13	120.42	111.48
85	3P	502	HEM	CHD-C1D-ND	4.12	128.85	124.42
69	1B	205	3PE	O21-C21-C22	4.11	120.38	111.48
69	3C	514	3PE	O21-C21-C22	4.11	120.37	111.48
75	3N	502	CDL	OA6-CA5-C11	4.11	120.37	111.48
69	3C	506	3PE	O21-C21-C22	4.11	120.37	111.48
70	1A	202	PC1	O21-C21-C22	4.11	120.37	111.48
75	4C	307	CDL	OB6-CB5-C51	4.10	120.36	111.48
86	3Q	501	HEC	CAA-CBA-CGA	-4.10	102.79	113.67
70	1H	404	PC1	O21-C21-C22	4.10	120.34	111.48
75	3X	103	CDL	OB6-CB5-C51	4.09	120.33	111.48
69	3C	507	3PE	O21-C21-C22	4.09	120.33	111.48
69	3Q	504	3PE	O21-C21-C22	4.06	120.27	111.48
91	4K	101	PGV	O01-C1-C2	4.06	120.26	111.48
69	1Y	215	3PE	O21-C21-C22	4.05	120.25	111.48
70	1h	202	PC1	O21-C21-C22	4.05	120.23	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	3A	502	3PE	O21-C21-C22	4.03	120.20	111.48
75	1Y	217	CDL	OB6-CB5-C51	4.03	120.20	111.48
69	1m	205	3PE	O21-C21-C22	4.03	120.19	111.48
69	3Y	103	3PE	O21-C21-C22	4.02	120.17	111.48
69	1Y	208	3PE	O21-C21-C22	4.01	120.16	111.48
69	1f	103	3PE	O21-C21-C22	4.01	120.16	111.48
69	1m	203	3PE	O21-C21-C22	4.01	120.15	111.48
88	4A	601	HEA	C2C-C1C-NC	4.01	116.56	110.14
88	4A	602	HEA	C2C-C1C-NC	4.01	116.56	110.14
69	3G	108	3PE	O21-C21-C22	4.00	120.13	111.48
75	1d	202	CDL	OA6-CA5-C11	3.99	120.12	111.48
88	4A	601	HEA	CHA-C4D-ND	-3.99	120.12	124.42
69	1b	101	3PE	O21-C21-C22	3.99	120.12	111.48
82	1Y	203	PGT	O2-C31-C32	3.99	120.12	111.48
91	4A	606	PGV	O01-C1-C2	3.99	120.11	111.48
69	3P	516	3PE	O21-C21-C22	3.99	120.11	111.48
69	3P	512	3PE	O21-C21-C22	3.99	120.11	111.48
69	3C	513	3PE	O21-C21-C22	3.97	120.07	111.48
69	1J	201	3PE	O21-C21-C22	3.97	120.06	111.48
69	1f	101	3PE	O21-C21-C22	3.97	120.06	111.48
75	1g	201	CDL	OB6-CB5-C51	3.96	120.05	111.48
69	1h	204	3PE	O21-C21-C22	3.96	120.05	111.48
69	3C	511	3PE	O21-C21-C22	3.95	120.03	111.48
69	1Z	201	3PE	O21-C21-C22	3.95	120.02	111.48
75	1N	402	CDL	OA6-CA5-C11	3.94	120.02	111.48
91	4J	101	PGV	O01-C1-C2	3.94	120.01	111.48
70	1Y	202	PC1	O21-C21-C22	3.94	120.00	111.48
75	4B	302	CDL	OA6-CA5-C11	3.94	120.00	111.48
75	1d	205	CDL	OB6-CB5-C51	3.94	120.00	111.48
91	4C	301	PGV	O01-C1-C2	3.93	119.98	111.48
69	3G	101	3PE	O31-C31-C32	3.93	123.81	111.83
69	1L	705	3PE	O21-C21-C22	3.91	119.93	111.48
75	1q	202	CDL	OB6-CB5-C51	3.90	119.93	111.48
69	3P	518	3PE	O21-C21-C22	3.90	119.91	111.48
91	4C	302	PGV	O01-C1-C2	3.89	119.91	111.48
69	1l	204	3PE	O21-C21-C22	3.89	119.90	111.48
69	3N	501	3PE	O21-C21-C22	3.89	119.90	111.48
86	3D	501	HEC	C2B-C1B-NB	3.88	116.37	110.14
75	1H	401	CDL	OA6-CA5-C11	3.88	119.87	111.48
91	4A	607	PGV	O01-C1-C2	3.87	119.86	111.48
69	1L	706	3PE	O21-C21-C22	3.87	119.85	111.48
69	3C	503	3PE	O21-C21-C22	3.86	119.83	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	4A	601	HEA	C13-C14-C15	-3.86	118.79	127.62
85	3P	502	HEM	CHA-C4D-ND	3.86	129.14	124.37
69	1Y	212	3PE	O21-C21-C22	3.85	119.82	111.48
91	4A	609	PGV	O01-C1-C2	3.85	119.81	111.48
69	1Y	213	3PE	O21-C21-C22	3.84	119.79	111.48
69	3J	104	3PE	O21-C21-C22	3.82	119.74	111.48
91	4A	608	PGV	O01-C1-C2	3.82	119.74	111.48
69	1f	104	3PE	O21-C21-C22	3.82	119.74	111.48
88	4A	601	HEA	C1D-C2D-C3D	-3.81	102.97	106.98
69	3P	520	3PE	O21-C21-C22	3.81	119.73	111.48
69	1L	702	3PE	O21-C21-C22	3.81	119.73	111.48
75	4C	306	CDL	OA6-CA5-C11	3.81	119.73	111.48
75	3T	101	CDL	OB6-CB5-C51	3.81	119.72	111.48
69	3P	505	3PE	O21-C21-C22	3.80	119.70	111.48
88	4A	601	HEA	C13-C12-C11	-3.79	108.34	114.39
69	3S	201	3PE	O21-C21-C22	3.79	119.68	111.48
69	3X	106	3PE	O21-C21-C22	3.79	119.67	111.48
93	4B	303	PSC	O01-C1-C2	3.79	119.67	111.48
69	3G	107	3PE	O21-C21-C22	3.78	119.65	111.48
69	3N	503	3PE	O21-C21-C22	3.78	119.65	111.48
69	3P	514	3PE	O21-C21-C22	3.78	119.65	111.48
69	1L	701	3PE	O31-C31-C32	3.78	123.35	111.83
69	3X	101	3PE	O21-C21-C22	3.77	119.65	111.48
69	3Y	104	3PE	O21-C21-C22	3.77	119.63	111.48
86	3Q	501	HEC	C1D-C2D-C3D	-3.77	102.50	106.82
69	1Y	204	3PE	O21-C21-C22	3.76	119.62	111.48
69	1Y	210	3PE	O21-C21-C22	3.75	119.60	111.48
69	3G	110	3PE	O21-C21-C22	3.75	119.59	111.48
69	3R	304	3PE	O21-C21-C22	3.75	119.59	111.48
69	3E	302	3PE	C2-O21-C21	-3.74	108.85	117.80
86	3D	501	HEC	C1D-C2D-C3D	-3.74	102.54	106.82
69	3W	102	3PE	O21-C21-C22	3.74	119.56	111.48
69	3G	105	3PE	O21-C21-C22	3.73	119.54	111.48
69	1J	203	3PE	O21-C21-C22	3.72	119.53	111.48
69	3G	102	3PE	O21-C21-C22	3.72	119.52	111.48
69	1Y	214	3PE	O21-C21-C22	3.72	119.52	111.48
69	4G	104	3PE	O21-C21-C22	3.71	119.51	111.48
91	4C	305	PGV	O01-C1-C2	3.71	119.51	111.48
86	3D	501	HEC	C2C-C1C-NC	3.71	116.09	110.14
75	1L	704	CDL	OA6-CA5-C11	3.71	119.50	111.48
69	1Y	211	3PE	C2-O21-C21	-3.70	108.94	117.80
69	3P	519	3PE	O21-C21-C22	3.70	119.49	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	4A	609	PGV	C02-O01-C1	-3.69	108.96	117.80
69	3W	101	3PE	O21-C21-C22	3.69	119.47	111.48
69	3Y	101	3PE	O21-C21-C22	3.69	119.47	111.48
70	1Y	206	PC1	O21-C21-C22	3.69	119.46	111.48
69	3G	101	3PE	C2-O21-C21	-3.68	108.99	117.80
69	1Y	201	3PE	O21-C21-C22	3.68	119.43	111.48
85	3C	502	HEM	CHA-C4D-ND	3.67	128.91	124.37
70	3T	102	PC1	O21-C21-C22	3.66	119.41	111.48
69	3Y	102	3PE	O21-C21-C22	3.66	119.41	111.48
86	3Q	501	HEC	C2B-C1B-NB	3.66	116.01	110.14
69	1d	201	3PE	O21-C21-C22	3.66	119.40	111.48
69	3C	510	3PE	O31-C31-C32	3.64	122.94	111.83
85	3P	502	HEM	C1B-NB-C4B	3.64	109.51	105.21
69	3G	111	3PE	O21-C21-C22	3.63	119.33	111.48
85	3C	502	HEM	CHB-C1B-NB	3.63	128.85	124.37
69	3T	103	3PE	O21-C21-C22	3.61	119.29	111.48
69	3G	109	3PE	O21-C21-C22	3.61	119.29	111.48
69	3P	510	3PE	O21-C21-C22	3.61	119.29	111.48
69	3N	503	3PE	C2-O21-C21	-3.61	109.16	117.80
85	3C	502	HEM	C1B-NB-C4B	3.61	109.48	105.21
69	3C	510	3PE	O21-C21-O22	-3.61	115.27	123.70
69	3J	103	3PE	O21-C21-C22	3.60	119.27	111.48
69	1Y	209	3PE	O21-C21-C22	3.59	119.25	111.48
69	1o	201	3PE	C2-O21-C21	-3.58	109.23	117.80
85	3P	502	HEM	CHB-C1B-NB	3.57	128.79	124.37
70	1B	202	PC1	C2-O21-C21	-3.57	109.25	117.80
69	3G	106	3PE	O21-C21-C22	3.57	119.20	111.48
69	3C	517	3PE	O21-C21-C22	3.56	119.19	111.48
75	3N	502	CDL	OB6-CB5-C51	3.56	119.18	111.48
88	4A	601	HEA	CAD-C3D-C4D	3.56	130.90	124.70
85	3C	501	HEM	C1B-NB-C4B	3.56	109.42	105.21
69	3Y	105	3PE	O21-C21-C22	3.55	119.16	111.48
88	4A	601	HEA	C1B-C2B-C3B	-3.55	102.69	106.80
75	1q	202	CDL	CA4-OA6-CA5	-3.55	109.31	117.80
86	3Q	501	HEC	C2C-C1C-NC	3.54	115.82	110.14
75	1H	401	CDL	OB6-CB5-C51	3.54	119.14	111.48
69	1g	202	3PE	O21-C21-C22	3.54	119.13	111.48
70	3X	104	PC1	O21-C21-C22	3.52	119.10	111.48
69	3R	302	3PE	C2-O21-C21	-3.52	109.36	117.80
69	3X	108	3PE	O21-C21-C22	3.51	119.08	111.48
75	4C	306	CDL	OB6-CB5-C51	3.51	119.08	111.48
88	4A	602	HEA	C1B-C2B-C3B	-3.50	102.74	106.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1l	203	3PE	O21-C21-C22	3.50	119.06	111.48
69	3P	506	3PE	C2-O21-C21	-3.49	109.43	117.80
69	1L	709	3PE	O31-C31-C32	3.48	122.43	111.83
70	1P	502	PC1	O21-C21-C22	3.46	118.97	111.48
69	3A	503	3PE	O21-C21-C22	3.46	118.96	111.48
75	3Y	106	CDL	OA6-CA5-C11	3.46	118.96	111.48
91	4G	102	PGV	O01-C1-C2	3.45	118.94	111.48
69	1l	202	3PE	O31-C31-C32	3.44	122.34	111.83
88	4A	601	HEA	C3A-C2A-C1A	-3.44	103.79	107.05
69	3P	517	3PE	O21-C21-C22	3.44	118.93	111.48
69	1Y	211	3PE	O21-C21-C22	3.44	118.92	111.48
69	3A	502	3PE	C2-O21-C21	-3.44	109.57	117.80
70	3T	102	PC1	C2-O21-C21	-3.44	109.57	117.80
69	3P	508	3PE	O31-C31-C32	3.43	122.29	111.83
85	3P	501	HEM	C1B-NB-C4B	3.42	109.25	105.21
70	1B	203	PC1	C2-O21-C21	-3.42	109.62	117.80
86	3D	501	HEC	CAA-CBA-CGA	-3.40	104.64	113.67
69	3C	513	3PE	O31-C31-C32	3.40	122.20	111.83
69	1M	502	3PE	O21-C21-C22	3.40	118.83	111.48
69	3G	106	3PE	C2-O21-C21	-3.39	109.68	117.80
77	1O	401	GTP	C6-C5-N7	3.39	136.46	130.29
75	1H	401	CDL	CB4-OB6-CB5	-3.39	109.69	117.80
75	3D	504	CDL	OB6-CB5-C51	3.38	118.79	111.48
70	3P	509	PC1	C2-O21-C21	-3.37	109.73	117.80
88	4A	601	HEA	C4D-C3D-C2D	-3.35	102.01	106.89
75	1L	704	CDL	OA8-CA7-C31	3.35	122.05	111.83
69	3X	105	3PE	O21-C21-C22	3.32	118.66	111.48
70	1H	403	PC1	O21-C21-C22	3.31	118.65	111.48
75	3T	101	CDL	CA4-OA6-CA5	-3.31	109.88	117.80
69	3P	507	3PE	O31-C31-C32	3.30	121.91	111.83
69	1L	707	3PE	O31-C31-C32	3.30	121.90	111.83
75	1d	202	CDL	OA8-CA7-C31	3.30	121.90	111.83
69	3P	507	3PE	O21-C21-C22	3.29	118.59	111.48
86	3Q	501	HEC	C4A-C3A-C2A	-3.28	102.11	106.97
69	3J	102	3PE	C2-O21-C21	-3.28	109.95	117.80
87	3X	102	PEK	O01-C1-C2	3.27	118.56	111.48
69	1f	102	3PE	O21-C21-C22	3.26	118.54	111.48
75	1L	704	CDL	OB8-CB7-C71	3.26	121.78	111.83
85	3C	501	HEM	CHA-C4D-ND	3.26	128.40	124.37
86	3D	501	HEC	C3A-C4A-NA	3.26	115.66	109.64
88	4A	602	HEA	C4A-NA-C1A	-3.26	100.51	105.82
85	3C	501	HEM	CHB-C1B-NB	3.24	128.38	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1L	702	3PE	O31-C31-C32	3.22	121.67	111.83
75	1g	201	CDL	OB8-CB7-C71	3.22	121.66	111.83
85	3P	501	HEM	CHA-C4D-ND	3.21	128.34	124.37
75	3T	101	CDL	OB8-CB7-C71	3.20	121.61	111.83
69	1L	711	3PE	O21-C21-C22	3.20	118.41	111.48
69	3D	503	3PE	O31-C31-C32	3.20	121.59	111.83
69	3P	506	3PE	O21-C21-C22	3.20	118.40	111.48
86	3D	501	HEC	C2D-C1D-ND	3.20	115.27	110.14
69	1m	201	3PE	O21-C21-C22	3.20	118.40	111.48
75	1i	201	CDL	OA8-CA7-C31	3.19	121.55	111.83
69	3P	518	3PE	C2-O21-C21	-3.18	110.17	117.80
75	3A	501	CDL	CB4-OB6-CB5	-3.18	110.19	117.80
70	1H	402	PC1	O31-C31-C32	3.18	121.53	111.83
70	1H	404	PC1	C11-C12-N	-3.18	105.63	115.82
69	3C	508	3PE	O31-C31-C32	3.16	121.48	111.83
75	3X	103	CDL	OB8-CB7-C71	3.16	121.47	111.83
70	1Y	207	PC1	C2-O21-C21	-3.15	110.25	117.80
86	3D	501	HEC	C4A-C3A-C2A	-3.15	102.29	106.97
69	1b	101	3PE	C2-O21-C21	-3.15	110.25	117.80
75	1q	201	CDL	OA8-CA7-C31	3.15	121.44	111.83
69	4G	104	3PE	O31-C31-C32	3.15	121.44	111.83
75	4C	307	CDL	CB4-OB6-CB5	-3.14	110.28	117.80
69	3T	103	3PE	O31-C31-C32	3.14	121.41	111.83
70	3R	303	PC1	O31-C31-C32	3.14	121.40	111.83
88	4A	601	HEA	C4A-NA-C1A	-3.13	100.72	105.82
88	4A	601	HEA	C4B-C3B-C2B	-3.13	102.17	107.44
88	4A	602	HEA	C4D-C3D-C2D	-3.13	102.33	106.89
69	3D	503	3PE	C2-O21-C21	-3.13	110.31	117.80
88	4A	601	HEA	C26-C15-C16	3.13	120.65	115.23
69	1L	710	3PE	O31-C31-C32	3.12	121.35	111.83
75	3D	504	CDL	OA8-CA7-C31	3.12	121.34	111.83
69	3X	107	3PE	O31-C31-C32	3.11	121.33	111.83
69	1Y	205	3PE	O21-C21-C22	3.11	118.21	111.48
85	3P	502	HEM	C3B-C4B-NB	-3.11	107.24	109.47
75	1g	201	CDL	OA6-CA5-C11	3.10	118.19	111.48
69	3C	507	3PE	O31-C31-C32	3.10	121.28	111.83
87	3X	102	PEK	O03-C21-C22	3.09	121.26	111.83
69	1f	103	3PE	O31-C31-C32	3.09	121.25	111.83
69	1m	204	3PE	C2-O21-C21	-3.08	110.41	117.80
88	4A	602	HEA	C4B-C3B-C2B	-3.08	102.26	107.44
75	1N	402	CDL	OB8-CB7-C71	3.08	121.23	111.83
69	1l	203	3PE	O31-C31-C32	3.08	121.23	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	3Q	501	HEC	C3A-C4A-NA	3.07	115.32	109.64
69	1L	708	3PE	O31-C31-C32	3.07	121.19	111.83
69	3P	506	3PE	O31-C31-C32	3.07	121.19	111.83
69	1Y	213	3PE	C2-O21-C21	-3.06	110.47	117.80
86	3D	501	HEC	C1A-C2A-C3A	-3.06	103.08	107.11
75	3T	101	CDL	CB4-OB6-CB5	-3.06	110.48	117.80
91	4C	303	PGV	O01-C1-C2	3.05	118.07	111.48
85	3C	502	HEM	C3B-C4B-NB	-3.05	107.28	109.47
69	3C	510	3PE	O21-C2-C1	-3.03	97.46	108.34
88	4A	602	HEA	C13-C14-C15	-3.03	120.69	127.62
86	3Q	501	HEC	C2D-C1D-ND	3.03	115.00	110.14
69	3Y	103	3PE	C2-O21-C21	-3.03	110.55	117.80
75	1Y	217	CDL	OA6-CA5-C11	3.02	118.02	111.48
70	1A	202	PC1	O31-C31-C32	3.02	121.04	111.83
69	1Y	215	3PE	C2-O21-C21	-3.02	110.57	117.80
69	3C	506	3PE	C2-O21-C21	-3.02	110.57	117.80
69	1g	202	3PE	O31-C31-C32	3.02	121.03	111.83
69	1A	201	3PE	C2-O21-C21	-3.01	110.58	117.80
70	1h	203	PC1	O31-C31-C32	3.01	121.01	111.83
75	1i	201	CDL	CA4-OA6-CA5	-3.01	110.59	117.80
69	1A	203	3PE	C2-O21-C21	-3.00	110.61	117.80
91	4A	606	PGV	O03-C19-C20	3.00	120.98	111.83
75	1q	201	CDL	OB8-CB7-C71	3.00	120.98	111.83
69	3G	106	3PE	O31-C31-C32	3.00	120.97	111.83
69	1f	104	3PE	C2-O21-C21	-3.00	110.62	117.80
75	3Y	106	CDL	OB8-CB7-C71	2.99	120.96	111.83
70	1Y	207	PC1	O31-C31-C32	2.99	120.95	111.83
69	3R	302	3PE	O31-C31-C32	2.99	120.94	111.83
69	3P	505	3PE	O31-C31-C32	2.99	120.94	111.83
69	1L	705	3PE	O31-C31-C32	2.99	120.94	111.83
85	3P	501	HEM	CHB-C1B-NB	2.98	128.06	124.37
70	1H	404	PC1	O31-C31-C32	2.98	120.93	111.83
69	3X	107	3PE	O21-C21-C22	2.98	117.92	111.48
75	3N	502	CDL	OA8-CA7-C31	2.97	120.90	111.83
75	4C	306	CDL	CA4-OA6-CA5	-2.97	110.68	117.80
75	1d	202	CDL	OB8-CB7-C71	2.97	120.89	111.83
69	1m	205	3PE	O31-C31-C32	2.97	120.89	111.83
69	3Q	504	3PE	C2-O21-C21	-2.97	110.69	117.80
69	3C	515	3PE	O31-C31-C32	2.97	120.88	111.83
69	3G	110	3PE	O31-C31-C32	2.97	120.88	111.83
91	4J	101	PGV	C02-O01-C1	-2.96	110.71	117.80
70	1P	502	PC1	O31-C31-C32	2.96	120.85	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	1l	204	3PE	O31-C31-C32	2.96	120.85	111.83
69	3G	102	3PE	O31-C31-C32	2.95	120.83	111.83
69	3Q	504	3PE	O31-C31-C32	2.95	120.83	111.83
70	1J	202	PC1	C2-O21-C21	-2.94	110.75	117.80
85	3P	501	HEM	CHD-C1D-C2D	-2.94	120.38	125.03
69	3C	516	3PE	O31-C31-C32	2.94	120.80	111.83
69	3E	303	3PE	O31-C31-C32	2.94	120.79	111.83
69	1A	201	3PE	O31-C31-C32	2.93	120.78	111.83
91	4A	608	PGV	O03-C19-C20	2.93	120.77	111.83
69	3Y	104	3PE	O31-C31-C32	2.93	120.76	111.83
75	1L	704	CDL	CA4-OA6-CA5	-2.93	110.79	117.80
69	1k	101	3PE	O31-C31-C32	2.93	120.75	111.83
69	3P	510	3PE	O31-C31-C32	2.92	120.75	111.83
69	3Y	105	3PE	O31-C31-C32	2.92	120.74	111.83
70	3X	104	PC1	O31-C31-C32	2.92	120.73	111.83
69	3E	302	3PE	O31-C31-C32	2.92	120.73	111.83
75	4C	307	CDL	OA6-CA5-C11	2.91	117.79	111.48
75	1q	202	CDL	OB8-CB7-C71	2.91	120.72	111.83
69	1L	701	3PE	O31-C31-O32	-2.91	116.34	123.63
70	3J	106	PC1	O31-C31-C32	2.91	120.72	111.83
87	4G	103	PEK	O03-C21-C22	2.91	120.70	111.83
88	4A	602	HEA	C13-C12-C11	-2.91	109.75	114.39
75	3D	504	CDL	CB4-OB6-CB5	-2.91	110.84	117.80
69	1Z	201	3PE	O31-C31-C32	2.91	120.69	111.83
69	3G	109	3PE	O31-C31-C32	2.90	120.69	111.83
69	3G	105	3PE	C2-O21-C21	-2.90	110.85	117.80
69	3W	102	3PE	O31-C31-C32	2.90	120.68	111.83
75	3P	513	CDL	CA4-OA6-CA5	-2.90	110.86	117.80
91	4A	609	PGV	O03-C19-C20	2.89	120.65	111.83
75	1i	201	CDL	OB8-CB7-C71	2.89	120.64	111.83
75	4C	306	CDL	OA8-CA7-C31	2.89	120.64	111.83
69	3P	508	3PE	C3-C2-C1	-2.89	105.05	111.78
93	4B	303	PSC	C02-O01-C1	-2.88	110.89	117.80
69	1J	203	3PE	O31-C31-C32	2.88	120.62	111.83
75	1q	201	CDL	CB4-OB6-CB5	-2.88	110.90	117.80
69	1Y	204	3PE	C2-O21-C21	-2.88	110.91	117.80
86	3Q	501	HEC	C1A-C2A-C3A	-2.88	103.32	107.11
69	3G	101	3PE	O31-C31-O32	-2.87	116.44	123.63
91	4C	305	PGV	O03-C19-C20	2.87	120.59	111.83
69	3N	503	3PE	O31-C31-C32	2.87	120.59	111.83
69	3P	517	3PE	O31-C31-C32	2.87	120.58	111.83
75	1d	202	CDL	OB8-CB7-OB9	-2.87	116.45	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	3C	514	3PE	C2-O21-C21	-2.87	110.93	117.80
69	1L	711	3PE	O31-C31-C32	2.86	120.57	111.83
70	1B	203	PC1	C11-C12-N	-2.86	106.63	115.82
75	4C	306	CDL	OB8-CB7-C71	2.86	120.56	111.83
75	3D	504	CDL	OB8-CB7-C71	2.86	120.55	111.83
88	4A	602	HEA	OMA-CMA-C3A	-2.86	119.17	125.62
70	3R	303	PC1	C2-O21-C21	-2.85	110.97	117.80
70	3T	102	PC1	O31-C31-C32	2.85	120.53	111.83
69	3S	201	3PE	O31-C31-C32	2.85	120.52	111.83
69	3Y	103	3PE	O31-C31-C32	2.85	120.52	111.83
88	4A	601	HEA	CBA-CAA-C2A	-2.85	104.66	112.53
69	3G	108	3PE	O31-C31-C32	2.85	120.51	111.83
70	3X	104	PC1	C2-O21-C21	-2.85	110.98	117.80
69	1f	102	3PE	C2-O21-C21	-2.84	110.99	117.80
70	3J	106	PC1	C2-O21-C21	-2.83	111.03	117.80
69	1L	705	3PE	C23-C22-C21	-2.82	103.37	113.69
69	3C	511	3PE	O31-C31-C32	2.81	120.40	111.83
69	1Z	201	3PE	C2-O21-C21	-2.81	111.08	117.80
69	1Y	208	3PE	C2-O21-C21	-2.80	111.08	117.80
69	3Q	503	3PE	O31-C31-C32	2.80	120.37	111.83
70	1d	204	PC1	C11-C12-N	-2.80	106.84	115.82
69	3A	502	3PE	O31-C31-C32	2.80	120.37	111.83
87	4G	103	PEK	C02-O01-C1	-2.80	111.10	117.80
70	1B	202	PC1	O31-C31-C32	2.80	120.36	111.83
75	1g	201	CDL	OA8-CA7-C31	2.80	120.36	111.83
75	3A	501	CDL	OA8-CA7-C31	2.79	120.35	111.83
69	1L	703	3PE	O31-C31-C32	2.79	120.34	111.83
83	1h	201	AME	O-C-CA	-2.79	117.60	124.77
75	3D	504	CDL	CA4-OA6-CA5	-2.79	111.12	117.80
75	1Y	217	CDL	OA8-CA7-C31	2.79	120.33	111.83
69	1Y	201	3PE	O31-C31-C32	2.79	120.33	111.83
75	1H	401	CDL	OA8-CA7-C31	2.79	120.33	111.83
91	4G	102	PGV	O03-C19-C20	2.78	120.32	111.83
69	1Y	211	3PE	O31-C31-C32	2.78	120.31	111.83
70	1Y	206	PC1	C2-O21-C21	-2.77	111.16	117.80
75	3Y	106	CDL	OA8-CA7-C31	2.77	120.29	111.83
70	1d	204	PC1	O31-C31-C32	2.77	120.28	111.83
91	4C	301	PGV	O03-C19-C20	2.77	120.28	111.83
75	1d	205	CDL	OA8-CA7-C31	2.77	120.28	111.83
69	1o	201	3PE	O31-C31-C32	2.77	120.28	111.83
70	1Y	206	PC1	O31-C31-C32	2.77	120.28	111.83
69	3P	507	3PE	O31-C31-O32	-2.77	116.71	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	4G	104	3PE	C2-O21-C21	-2.77	111.17	117.80
70	3J	106	PC1	C11-C12-N	-2.76	106.95	115.82
69	1m	203	3PE	C2-O21-C21	-2.76	111.19	117.80
82	1Y	203	PGT	O3-C11-C12	2.76	120.25	111.83
75	1d	202	CDL	CA4-OA6-CA5	-2.76	111.20	117.80
69	1M	502	3PE	O31-C31-C32	2.76	120.24	111.83
75	1d	202	CDL	CB6-CB4-CB3	-2.75	105.36	111.78
75	4B	302	CDL	OB8-CB7-C71	2.75	120.23	111.83
75	4C	306	CDL	CB4-OB6-CB5	-2.75	111.21	117.80
69	3A	503	3PE	O31-C31-C32	2.75	120.22	111.83
77	1O	401	GTP	O4'-C1'-N9	2.75	114.59	108.36
69	1Y	201	3PE	C2-O21-C21	-2.75	111.22	117.80
69	1Y	212	3PE	O31-C31-C32	2.74	120.20	111.83
75	3F	201	CDL	OB8-CB7-C71	2.74	120.19	111.83
69	1e	201	3PE	C2-O21-C21	-2.74	111.25	117.80
69	1f	102	3PE	O31-C31-C32	2.74	120.18	111.83
69	1h	204	3PE	O31-C31-C32	2.74	120.18	111.83
69	1B	204	3PE	O31-C31-C32	2.74	120.18	111.83
70	1B	203	PC1	O31-C31-C32	2.74	120.18	111.83
69	1J	201	3PE	O31-C31-C32	2.73	120.17	111.83
69	3G	103	3PE	O31-C31-C32	2.73	120.15	111.83
85	3C	501	HEM	CHD-C1D-C2D	-2.72	120.73	125.03
69	1Y	209	3PE	O31-C31-C32	2.72	120.14	111.83
69	1g	203	3PE	O31-C31-C32	2.72	120.13	111.83
69	3C	506	3PE	O31-C31-C32	2.72	120.13	111.83
69	3P	516	3PE	O31-C31-C32	2.72	120.13	111.83
69	1d	206	3PE	O31-C31-C32	2.72	120.13	111.83
69	1f	104	3PE	O31-C31-C32	2.72	120.12	111.83
86	3D	501	HEC	CBB-CAB-C3B	-2.72	122.00	127.43
69	1m	203	3PE	O31-C31-C32	2.71	120.11	111.83
69	3X	105	3PE	O31-C31-C32	2.71	120.10	111.83
69	1L	706	3PE	O31-C31-C32	2.71	120.10	111.83
69	3G	111	3PE	O31-C31-C32	2.71	120.10	111.83
69	3P	512	3PE	C2-O21-C21	-2.71	111.31	117.80
86	3Q	501	HEC	CMD-C2D-C1D	2.71	129.54	125.42
69	3R	304	3PE	O31-C31-C32	2.71	120.09	111.83
88	4A	602	HEA	C26-C15-C16	2.70	119.92	115.23
69	1L	709	3PE	C2-O21-C21	-2.70	111.33	117.80
75	3X	103	CDL	OA8-CA7-C31	2.70	120.08	111.83
88	4A	602	HEA	C27-C19-C20	2.70	119.92	115.23
69	3C	517	3PE	O31-C31-C32	2.70	120.07	111.83
69	1Y	214	3PE	C2-O21-C21	-2.70	111.33	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	3P	509	PC1	O31-C31-C32	2.70	120.06	111.83
69	1l	204	3PE	C2-O21-C21	-2.70	111.34	117.80
69	1d	203	3PE	O31-C31-C32	2.69	120.05	111.83
70	1M	501	PC1	O31-C31-C32	2.69	120.05	111.83
69	3N	501	3PE	O31-C31-C32	2.69	120.03	111.83
75	1Y	217	CDL	OB8-CB7-C71	2.69	120.03	111.83
69	1m	204	3PE	O31-C31-C32	2.68	120.01	111.83
88	4A	602	HEA	CHA-C4D-ND	-2.68	121.54	124.42
69	3X	101	3PE	O31-C31-C32	2.68	120.00	111.83
69	1d	206	3PE	O21-C21-C22	2.68	117.27	111.48
69	3X	108	3PE	O31-C31-C32	2.67	119.99	111.83
69	3C	512	3PE	O31-C31-C32	2.67	119.98	111.83
69	1f	103	3PE	C2-O21-C21	-2.67	111.40	117.80
69	1B	205	3PE	O31-C31-C32	2.67	119.98	111.83
91	4A	607	PGV	O03-C19-C20	2.67	119.96	111.83
69	1N	401	3PE	C2-O21-C21	-2.66	111.43	117.80
69	1Y	205	3PE	O31-C31-C32	2.66	119.93	111.83
91	4C	302	PGV	O03-C19-C20	2.65	119.93	111.83
69	3G	107	3PE	O31-C31-C32	2.65	119.92	111.83
75	1H	401	CDL	OB8-CB7-C71	2.65	119.92	111.83
75	3T	101	CDL	OA8-CA7-C31	2.65	119.90	111.83
75	3F	201	CDL	OA8-CA7-C31	2.64	119.89	111.83
70	1M	501	PC1	C11-C12-N	-2.64	107.35	115.82
69	3P	511	3PE	C2-O21-C21	-2.63	111.49	117.80
69	1Y	216	3PE	O31-C31-C32	2.63	119.87	111.83
69	3N	501	3PE	C2-O21-C21	-2.63	111.49	117.80
69	3P	520	3PE	C2-O21-C21	-2.63	111.50	117.80
69	1d	201	3PE	O31-C31-C32	2.63	119.86	111.83
75	4B	302	CDL	OA8-CA7-C31	2.63	119.84	111.83
91	4C	304	PGV	O03-C19-C20	2.62	119.83	111.83
70	1Y	202	PC1	O31-C31-C32	2.62	119.81	111.83
70	1h	202	PC1	O31-C31-C32	2.61	119.81	111.83
75	1N	402	CDL	CB4-OB6-CB5	-2.61	111.54	117.80
69	1Y	213	3PE	O31-C31-C32	2.61	119.79	111.83
70	1H	403	PC1	O31-C31-C32	2.61	119.78	111.83
69	1Y	216	3PE	C3-C2-C1	-2.61	105.71	111.78
75	4C	307	CDL	OA8-CA7-C31	2.60	119.77	111.83
91	4N	101	PGV	C02-O01-C1	-2.60	111.57	117.80
69	3Y	107	3PE	O31-C31-C32	2.60	119.76	111.83
75	1d	205	CDL	OB8-CB7-C71	2.60	119.76	111.83
70	1H	404	PC1	C2-O21-C21	-2.60	111.57	117.80
91	4N	101	PGV	O03-C19-C20	2.60	119.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	3P	505	3PE	C2-O21-C21	-2.60	111.58	117.80
88	4A	602	HEA	C1D-ND-C4D	-2.60	102.13	105.21
69	3P	508	3PE	O21-C21-O22	-2.59	117.65	123.70
69	3P	520	3PE	O31-C31-C32	2.59	119.73	111.83
69	1L	712	3PE	O31-C31-C32	2.59	119.73	111.83
69	3J	101	3PE	O31-C31-C32	2.59	119.72	111.83
70	1B	202	PC1	C24-C23-C22	2.58	122.62	113.13
70	1d	204	PC1	C3-C2-C1	-2.58	105.77	111.78
69	3P	503	3PE	O31-C31-C32	2.58	119.71	111.83
69	1J	201	3PE	C2-O21-C21	-2.58	111.62	117.80
69	1Y	204	3PE	O31-C31-C32	2.58	119.69	111.83
77	1O	401	GTP	C2'-C1'-N9	-2.58	106.08	113.25
69	3C	503	3PE	O31-C31-C32	2.58	119.69	111.83
93	4B	303	PSC	O03-C19-C20	2.57	119.68	111.83
86	3Q	501	HEC	CBD-CAD-C3D	-2.57	105.42	112.53
69	1Y	210	3PE	O31-C31-C32	2.57	119.67	111.83
91	4C	305	PGV	C02-O01-C1	-2.57	111.64	117.80
88	4A	601	HEA	C27-C19-C20	2.57	119.69	115.23
69	1Y	208	3PE	O31-C31-C32	2.57	119.66	111.83
85	3P	501	HEM	CHD-C4C-NC	2.56	127.25	124.45
69	3W	103	3PE	C2-O21-C21	-2.56	111.66	117.80
86	3D	501	HEC	CMD-C2D-C1D	2.56	129.32	125.42
75	1q	202	CDL	OA8-CA7-C31	2.56	119.65	111.83
70	1J	202	PC1	O31-C31-C32	2.55	119.62	111.83
69	3C	514	3PE	O31-C31-C32	2.55	119.62	111.83
86	3Q	501	HEC	CBB-CAB-C3B	-2.55	122.33	127.43
75	3P	513	CDL	OB8-CB7-C71	2.55	119.62	111.83
69	4G	101	3PE	O31-C31-C32	2.55	119.60	111.83
69	3P	514	3PE	O31-C31-C32	2.54	119.59	111.83
85	3C	502	HEM	CHD-C1D-C2D	-2.54	121.02	125.03
91	4J	101	PGV	O03-C19-C20	2.54	119.58	111.83
79	1P	501	NDP	O4D-C1D-C2D	-2.54	101.19	106.62
69	3P	512	3PE	O31-C31-C32	2.53	119.56	111.83
86	3D	501	HEC	C4D-C3D-C2D	-2.53	102.95	106.87
69	1Y	209	3PE	C2-O21-C21	-2.53	111.75	117.80
69	3P	508	3PE	C2-O21-C21	-2.53	111.75	117.80
69	1e	201	3PE	O31-C31-C32	2.53	119.54	111.83
69	1L	710	3PE	C2-O21-C21	-2.52	111.76	117.80
75	4B	302	CDL	CB4-OB6-CB5	-2.52	111.76	117.80
69	3P	510	3PE	C2-O21-C21	-2.52	111.77	117.80
69	3P	518	3PE	O31-C31-C32	2.52	119.51	111.83
75	4C	307	CDL	OB8-CB7-C71	2.52	119.51	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	1N	402	CDL	OA8-CA7-C31	2.52	119.51	111.83
69	1L	701	3PE	C2-O21-C21	-2.51	111.78	117.80
69	1A	203	3PE	O31-C31-C32	2.51	119.49	111.83
85	3C	501	HEM	CHD-C4C-NC	2.51	127.18	124.45
88	4A	601	HEA	C4B-NB-C1B	-2.51	102.24	105.21
88	4A	601	HEA	C17-C18-C19	-2.51	121.89	127.62
69	1L	702	3PE	C2-O21-C21	-2.51	111.80	117.80
91	4A	607	PGV	C02-O01-C1	-2.50	111.81	117.80
69	1N	401	3PE	O31-C31-C32	2.50	119.46	111.83
69	1o	201	3PE	O21-C21-O22	-2.50	117.86	123.70
69	3P	515	3PE	O31-C31-C32	2.50	119.46	111.83
69	3C	509	3PE	O31-C31-C32	2.49	119.42	111.83
75	3P	513	CDL	C32-C31-CA7	-2.48	104.59	113.69
75	3P	513	CDL	OB6-CB5-OB7	-2.48	117.91	123.70
91	4C	302	PGV	C02-O01-C1	-2.48	111.86	117.80
86	3Q	501	HEC	CMA-C3A-C4A	2.48	129.09	124.73
69	3Y	102	3PE	O31-C31-C32	2.47	119.37	111.83
75	1L	704	CDL	OB8-CB7-OB9	-2.47	117.46	123.63
69	1m	201	3PE	O31-C31-C32	2.46	119.33	111.83
88	4A	601	HEA	C1D-ND-C4D	-2.46	102.30	105.21
69	1m	202	3PE	O31-C31-C32	2.46	119.32	111.83
69	1L	707	3PE	O31-C31-O32	-2.45	117.49	123.63
69	3P	515	3PE	O21-C21-O22	-2.45	117.98	123.70
85	3C	501	HEM	C3B-C4B-NB	-2.45	107.71	109.47
69	3P	504	3PE	O31-C31-C32	2.45	119.29	111.83
69	3Y	101	3PE	O31-C31-C32	2.44	119.29	111.83
69	1b	101	3PE	O31-C31-C32	2.44	119.28	111.83
69	3G	105	3PE	O31-C31-C32	2.44	119.28	111.83
86	3Q	501	HEC	C4D-C3D-C2D	-2.44	103.09	106.87
69	3G	101	3PE	O21-C21-O22	-2.43	118.02	123.70
69	3E	303	3PE	C2-O21-C21	-2.43	111.97	117.80
88	4A	601	HEA	CHC-C1C-C2C	-2.43	120.37	127.43
70	1d	204	PC1	O31-C31-O32	-2.43	117.56	123.63
75	1q	201	CDL	OA8-CA7-OA9	-2.43	117.56	123.63
69	3Q	502	3PE	O31-C31-C32	2.43	119.23	111.83
75	3P	513	CDL	CB6-CB4-CB3	-2.42	106.14	111.78
69	3C	508	3PE	O31-C31-O32	-2.42	117.58	123.63
85	3C	502	HEM	CHD-C4C-NC	2.42	127.08	124.45
69	3G	104	3PE	O31-C31-C32	2.42	119.20	111.83
86	3D	501	HEC	CBC-CAC-C3C	-2.41	122.61	127.43
91	4G	102	PGV	C02-O01-C1	-2.41	112.02	117.80
69	3J	105	3PE	O31-C31-C32	2.41	119.18	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	4C	303	PGV	O03-C19-C20	2.41	119.18	111.83
77	1O	401	GTP	C4-C5-N7	-2.41	106.85	110.67
91	4K	101	PGV	O03-C19-C20	2.41	119.18	111.83
69	3P	516	3PE	C2-O21-C21	-2.41	112.03	117.80
70	1A	202	PC1	C2-O21-C21	-2.41	112.03	117.80
70	3R	303	PC1	O21-C21-O22	-2.41	118.08	123.70
69	3P	508	3PE	O31-C31-O32	-2.40	117.62	123.63
70	3J	106	PC1	O31-C31-O32	-2.40	117.62	123.63
70	3P	509	PC1	C11-C12-N	-2.40	108.13	115.82
69	1g	202	3PE	C2-O21-C21	-2.40	112.06	117.80
69	3R	305	3PE	O31-C31-O32	-2.40	117.64	123.63
88	4A	601	HEA	CHB-C1B-C2B	-2.39	121.25	125.03
75	1i	201	CDL	OA8-CA7-OA9	-2.39	117.65	123.63
69	3G	109	3PE	C2-O21-C21	-2.39	112.08	117.80
69	3X	101	3PE	C2-O21-C21	-2.38	112.10	117.80
69	1L	708	3PE	O31-C31-O32	-2.38	117.67	123.63
70	1H	404	PC1	P-O13-C11	-2.38	109.94	121.26
91	4C	304	PGV	C02-O01-C1	-2.38	112.11	117.80
69	3G	101	3PE	C33-C32-C31	-2.38	104.99	113.69
75	1i	201	CDL	CB6-CB4-CB3	-2.37	106.25	111.78
69	3C	505	3PE	C2-O21-C21	-2.37	112.12	117.80
69	3C	512	3PE	C2-O21-C21	-2.37	112.13	117.80
69	1Y	215	3PE	O31-C31-C32	2.37	119.06	111.83
69	1k	101	3PE	O31-C31-O32	-2.37	117.70	123.63
88	4A	602	HEA	CHC-C1C-C2C	-2.37	120.56	127.43
75	3A	501	CDL	OB8-CB7-C71	2.37	119.05	111.83
70	1B	203	PC1	O21-C21-O22	-2.36	118.18	123.70
86	3Q	501	HEC	CBC-CAC-C3C	-2.36	122.72	127.43
69	1N	401	3PE	C3-C2-C1	-2.36	106.28	111.78
69	3R	302	3PE	O31-C31-O32	-2.36	117.73	123.63
91	4K	101	PGV	C02-O01-C1	-2.36	112.15	117.80
69	3D	503	3PE	O31-C31-O32	-2.36	117.73	123.63
88	4A	601	HEA	CHB-C1B-NB	-2.36	121.89	124.42
70	1B	202	PC1	O21-C21-O22	-2.36	118.20	123.70
70	3P	509	PC1	O21-C21-O22	-2.35	118.20	123.70
70	1Y	202	PC1	C2-O21-C21	-2.35	112.18	117.80
88	4A	601	HEA	CHA-C1A-NA	-2.34	121.90	124.45
69	3J	103	3PE	O31-C31-C32	2.34	118.98	111.83
69	3E	303	3PE	O21-C21-O22	-2.34	118.23	123.70
75	3N	502	CDL	OB8-CB7-C71	2.34	118.96	111.83
85	3P	501	HEM	CHA-C1A-NA	2.34	128.10	123.86
69	1L	705	3PE	C2-O21-C21	-2.33	112.21	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	4C	301	PGV	C02-O01-C1	-2.33	112.22	117.80
75	1g	201	CDL	OB8-CB7-OB9	-2.33	117.80	123.63
75	1L	704	CDL	OB6-CB5-OB7	-2.33	118.27	123.70
69	1J	203	3PE	C2-O21-C21	-2.32	112.23	117.80
87	3X	102	PEK	C3-C2-C1	-2.32	105.18	113.69
75	3N	502	CDL	CB4-OB6-CB5	-2.32	112.23	117.80
69	1N	401	3PE	O21-C21-O22	-2.32	118.28	123.70
69	3G	110	3PE	C2-O21-C21	-2.32	112.24	117.80
69	3C	514	3PE	O21-C21-O22	-2.32	118.28	123.70
88	4A	601	HEA	CMC-C2C-C1C	2.32	128.95	125.42
70	3X	104	PC1	O31-C31-O32	-2.31	117.84	123.63
75	1i	201	CDL	OB8-CB7-OB9	-2.31	117.84	123.63
69	3P	511	3PE	O31-C31-C32	2.31	118.89	111.83
88	4A	601	HEA	CMD-C2D-C1D	2.31	128.65	125.03
69	3W	101	3PE	O31-C31-C32	2.31	118.88	111.83
70	3J	106	PC1	C14-N-C13	2.31	115.04	108.98
69	1Y	216	3PE	C2-O21-C21	-2.30	112.28	117.80
85	3P	502	HEM	CHA-C4D-C3D	-2.30	120.98	125.23
85	3P	502	HEM	CHD-C1D-C2D	-2.30	121.39	125.03
88	4A	602	HEA	CMB-C2B-C1B	2.30	128.63	125.03
69	3C	509	3PE	C2-O21-C21	-2.30	112.29	117.80
88	4A	602	HEA	C25-C23-C24	2.30	119.88	114.59
69	3P	503	3PE	C2-O21-C21	-2.30	112.29	117.80
85	3P	502	HEM	CHD-C4C-NC	2.30	126.95	124.45
85	3C	502	HEM	O2A-CGA-CBA	2.30	121.25	114.00
69	1Y	214	3PE	O31-C31-C32	2.29	118.83	111.83
75	1q	202	CDL	OA6-CA5-OA7	-2.29	118.35	123.70
75	1d	205	CDL	OA6-CA5-OA7	-2.29	118.35	123.70
69	3C	505	3PE	O31-C31-C32	2.29	118.81	111.83
88	4A	601	HEA	CHD-C1D-C2D	-2.29	120.45	126.95
88	4A	602	HEA	C17-C18-C19	-2.28	122.40	127.62
69	1e	201	3PE	O21-C21-O22	-2.28	118.37	123.70
69	4G	101	3PE	O21-C21-O22	-2.28	118.37	123.70
86	3D	501	HEC	CHC-C1C-C2C	-2.28	120.80	127.43
75	1q	201	CDL	OA6-CA5-OA7	-2.28	118.38	123.70
87	4G	103	PEK	O03-C21-O04	-2.27	117.94	123.63
70	1H	403	PC1	C2-O21-C21	-2.27	112.36	117.80
69	3P	519	3PE	O31-C31-C32	2.27	118.76	111.83
69	3T	103	3PE	O31-C31-O32	-2.27	117.96	123.63
88	4A	601	HEA	C25-C23-C24	2.27	119.80	114.59
69	1l	202	3PE	C3-C2-C1	-2.26	106.50	111.78
86	3D	501	HEC	CHB-C1B-C2B	-2.26	120.86	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	3F	201	CDL	CB4-OB6-CB5	-2.26	112.38	117.80
86	3D	501	HEC	CMA-C3A-C4A	2.25	128.70	124.73
88	4A	602	HEA	CHB-C1B-NB	-2.25	122.00	124.42
85	3P	501	HEM	C1A-CHA-C4D	-2.25	120.96	126.25
69	1Y	209	3PE	C23-C22-C21	-2.25	105.46	113.69
88	4A	601	HEA	CMB-C2B-C1B	2.24	128.54	125.03
69	1A	201	3PE	O21-C21-O22	-2.24	118.46	123.70
69	3Y	105	3PE	C2-O21-C21	-2.24	112.43	117.80
69	1B	204	3PE	O21-C21-O22	-2.24	118.47	123.70
69	1f	101	3PE	O31-C31-C32	2.24	118.65	111.83
75	3D	504	CDL	OA8-CA7-OA9	-2.23	118.06	123.63
85	3P	501	HEM	C3B-C4B-NB	-2.23	107.87	109.47
69	1d	206	3PE	C23-C22-C21	-2.22	105.56	113.69
69	3J	104	3PE	O31-C31-C32	2.21	118.59	111.83
69	1l	202	3PE	O31-C31-O32	-2.21	118.10	123.63
69	4G	104	3PE	O31-C31-O32	-2.20	118.13	123.63
75	3T	101	CDL	CA6-CA4-CA3	-2.20	106.67	111.78
75	1H	401	CDL	CA4-OA6-CA5	-2.20	112.54	117.80
88	4A	602	HEA	CMC-C2C-C1C	2.19	128.76	125.42
75	3A	501	CDL	OA6-CA5-OA7	-2.19	118.58	123.70
69	3A	503	3PE	O31-C31-O32	-2.19	118.14	123.63
70	1H	402	PC1	O31-C31-O32	-2.19	118.14	123.63
88	4A	602	HEA	C4B-NB-C1B	-2.19	102.61	105.21
69	3J	104	3PE	C33-C32-C31	-2.19	105.67	113.69
88	4A	601	HEA	CAD-CBD-CGD	-2.19	107.86	113.67
85	3P	502	HEM	C1A-CHA-C4D	-2.19	121.11	126.25
70	1B	203	PC1	O31-C31-O32	-2.19	118.16	123.63
69	1L	701	3PE	C23-C22-C21	-2.18	105.70	113.69
88	4A	602	HEA	CHA-C4D-C3D	-2.18	121.59	124.77
85	3P	502	HEM	O2D-CGD-CBD	2.18	120.89	114.00
69	3E	302	3PE	O31-C31-O32	-2.18	118.17	123.63
69	1m	204	3PE	O21-C21-O22	-2.18	118.61	123.70
85	3C	502	HEM	C1A-CHA-C4D	-2.18	121.12	126.25
69	3Y	107	3PE	C2-O21-C21	-2.18	112.59	117.80
87	3X	102	PEK	C2-C3-C4	-2.17	108.61	113.35
69	3C	517	3PE	C2-O21-C21	-2.17	112.60	117.80
69	1L	702	3PE	O31-C31-O32	-2.17	118.20	123.63
85	3P	502	HEM	C4C-CHD-C1D	-2.17	121.41	126.02
69	3Y	102	3PE	C3-C2-C1	-2.16	106.74	111.78
75	3P	513	CDL	OA8-CA7-C31	2.16	118.43	111.83
70	1P	502	PC1	C2-O21-C21	-2.16	112.62	117.80
69	1Z	201	3PE	O21-C21-O22	-2.16	118.66	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
75	3F	201	CDL	OB6-CB5-OB7	-2.16	118.66	123.70
69	3R	305	3PE	O31-C31-C32	2.16	118.42	111.83
91	4A	608	PGV	C02-O01-C1	-2.15	112.64	117.80
69	1k	101	3PE	O21-C21-O22	-2.15	118.67	123.70
69	1L	707	3PE	C3-C2-C1	-2.15	106.76	111.78
69	1d	203	3PE	O21-C21-O22	-2.15	118.67	123.70
70	1h	202	PC1	C11-C12-N	-2.15	108.91	115.82
69	1B	204	3PE	C2-O21-C21	-2.15	112.65	117.80
85	3C	501	HEM	CHA-C1A-NA	2.15	127.76	123.86
69	3P	503	3PE	O21-C21-O22	-2.15	118.69	123.70
82	1Y	203	PGT	C2-O2-C31	-2.14	112.67	117.80
69	3C	511	3PE	C2-O21-C21	-2.14	112.67	117.80
75	1d	202	CDL	OA8-CA7-OA9	-2.14	118.28	123.63
69	3Y	103	3PE	O21-C21-O22	-2.14	118.70	123.70
88	4A	602	HEA	C1A-CHA-C4D	-2.14	121.48	126.02
69	3R	302	3PE	O21-C21-O22	-2.14	118.71	123.70
88	4A	601	HEA	CHC-C4B-NB	-2.14	121.73	124.37
69	1Y	215	3PE	O21-C21-O22	-2.13	118.71	123.70
69	1Y	210	3PE	C2-O21-C21	-2.13	112.69	117.80
75	4B	302	CDL	CA4-OA6-CA5	-2.13	112.69	117.80
75	3D	504	CDL	OB6-CB5-OB7	-2.13	118.72	123.70
88	4A	602	HEA	CMD-C2D-C1D	2.13	128.36	125.03
75	1L	704	CDL	OA8-CA7-OA9	-2.13	118.31	123.63
75	1Y	217	CDL	OA8-CA7-OA9	-2.12	118.32	123.63
75	3D	504	CDL	OA6-CA5-OA7	-2.12	118.75	123.70
88	4A	602	HEA	CHD-C1D-C2D	-2.12	120.93	126.95
69	3G	106	3PE	O21-C21-O22	-2.12	118.76	123.70
85	3C	502	HEM	CHA-C4D-C3D	-2.11	121.33	125.23
69	1g	202	3PE	O21-C21-O22	-2.11	118.77	123.70
69	3J	105	3PE	O21-C21-O22	-2.11	118.77	123.70
75	3A	501	CDL	CB6-CB4-CB3	-2.11	106.87	111.78
69	1m	202	3PE	C2-O21-C21	-2.11	112.76	117.80
70	1H	404	PC1	O31-C31-O32	-2.11	118.36	123.63
69	3X	107	3PE	O31-C31-O32	-2.10	118.36	123.63
69	3P	519	3PE	C3-C2-C1	-2.10	106.88	111.78
69	3C	506	3PE	O21-C21-O22	-2.10	118.80	123.70
69	3A	502	3PE	O31-C31-O32	-2.10	118.38	123.63
69	1L	709	3PE	O21-C21-O22	-2.10	118.80	123.70
85	3P	502	HEM	O2A-CGA-CBA	2.09	120.61	114.00
70	1A	202	PC1	O31-C31-O32	-2.09	118.39	123.63
70	3P	509	PC1	O31-C31-O32	-2.09	118.39	123.63
86	3Q	501	HEC	CMC-C2C-C3C	2.09	131.47	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	3P	502	HEM	C4D-ND-C1D	2.09	107.68	105.21
69	3C	513	3PE	O31-C31-O32	-2.09	118.40	123.63
69	3J	102	3PE	O21-C21-O22	-2.09	118.82	123.70
70	3T	102	PC1	O21-C21-O22	-2.09	118.83	123.70
85	3C	502	HEM	C4C-CHD-C1D	-2.09	121.58	126.02
69	3C	508	3PE	O21-C21-O22	-2.08	118.83	123.70
69	3G	104	3PE	O21-C21-O22	-2.08	118.83	123.70
86	3D	501	HEC	CMC-C2C-C3C	2.08	131.45	126.55
69	1g	203	3PE	C23-C22-C21	-2.08	106.07	113.69
69	3P	508	3PE	O13-C11-C12	-2.08	101.55	109.17
69	1B	205	3PE	O21-C21-O22	-2.08	118.84	123.70
77	1O	401	GTP	O6-C6-C5	-2.08	121.04	126.53
86	3Q	501	HEC	CHC-C1C-C2C	-2.08	121.39	127.43
91	4J	101	PGV	O01-C1-O02	-2.08	118.85	123.70
85	3P	502	HEM	C4A-CHB-C1B	-2.07	121.37	126.25
88	4A	602	HEA	C21-C22-C23	-2.07	120.73	127.64
75	1d	202	CDL	C12-C11-CA5	-2.07	106.10	113.69
75	3P	513	CDL	CA6-CA4-CA3	-2.07	106.95	111.78
88	4A	602	HEA	CHA-C1A-C2A	-2.07	121.59	124.86
69	3R	304	3PE	C2-O21-C21	-2.07	112.84	117.80
91	4A	606	PGV	O01-C1-O02	-2.07	118.86	123.70
69	3C	516	3PE	O21-C21-O22	-2.07	118.86	123.70
85	3C	501	HEM	C1A-CHA-C4D	-2.07	121.38	126.25
69	1A	201	3PE	O31-C31-O32	-2.07	118.46	123.63
75	1d	202	CDL	OA6-CA5-OA7	-2.07	118.87	123.70
69	1L	702	3PE	O21-C21-O22	-2.07	118.87	123.70
69	3J	104	3PE	C2-O21-C21	-2.06	112.86	117.80
88	4A	602	HEA	CHB-C1B-C2B	-2.06	121.77	125.03
69	3C	512	3PE	O21-C21-O22	-2.06	118.88	123.70
69	1g	202	3PE	O31-C31-O32	-2.06	118.47	123.63
73	1F	501	FMN	C4-N3-C2	-2.06	121.98	125.64
70	1B	202	PC1	C11-C12-N	-2.06	109.21	115.82
91	4C	304	PGV	O01-C1-O02	-2.06	118.89	123.70
75	1L	704	CDL	OA6-CA5-OA7	-2.05	118.91	123.70
75	3A	501	CDL	OB6-CB5-OB7	-2.05	118.91	123.70
75	1q	201	CDL	CA4-OA6-CA5	-2.05	112.89	117.80
69	1b	101	3PE	O21-C21-O22	-2.05	118.91	123.70
69	3P	519	3PE	C34-C33-C32	-2.05	105.60	113.13
69	3N	503	3PE	O21-C21-O22	-2.05	118.92	123.70
69	3C	505	3PE	O21-C21-O22	-2.05	118.92	123.70
69	3P	510	3PE	O21-C21-O22	-2.05	118.92	123.70
70	1h	203	PC1	C3-C2-C1	-2.04	107.02	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
70	3X	104	PC1	C23-C22-C21	-2.04	106.20	113.69
69	1Y	216	3PE	O31-C31-O32	-2.04	118.51	123.63
69	1o	201	3PE	O12-P-O14	2.04	121.95	112.44
75	1N	402	CDL	C32-C31-CA7	-2.04	106.21	113.69
69	3J	102	3PE	O31-C31-C32	2.04	118.06	111.83
70	1B	202	PC1	C3-C2-C1	-2.04	107.03	111.78
87	3X	102	PEK	O03-C21-O04	-2.04	118.52	123.63
75	4B	302	CDL	OB6-CB5-OB7	-2.04	118.94	123.70
85	3C	501	HEM	O2D-CGD-CBD	2.04	120.44	114.00
85	3C	502	HEM	CHB-C1B-C2B	-2.04	121.16	126.95
75	3X	103	CDL	OA6-CA5-OA7	-2.04	118.94	123.70
69	1L	707	3PE	C2-O21-C21	-2.04	112.92	117.80
69	1J	203	3PE	O21-C21-O22	-2.03	118.95	123.70
85	3P	501	HEM	O2A-CGA-CBA	2.03	120.43	114.00
93	4B	303	PSC	C04-C05-N	-2.03	109.29	115.82
69	3Y	104	3PE	O31-C31-O32	-2.03	118.55	123.63
70	1P	502	PC1	O31-C31-O32	-2.03	118.55	123.63
69	1m	205	3PE	C2-O21-C21	-2.03	112.94	117.80
85	3P	502	HEM	CHB-C1B-C2B	-2.03	121.18	126.95
75	3T	101	CDL	OB6-CB5-OB7	-2.03	118.96	123.70
85	3P	501	HEM	O2D-CGD-CBD	2.03	120.41	114.00
85	3C	501	HEM	O2A-CGA-CBA	2.03	120.41	114.00
75	3F	201	CDL	CA4-OA6-CA5	-2.03	112.95	117.80
75	1q	201	CDL	CA6-CA4-CA3	-2.03	107.06	111.78
69	3C	514	3PE	O31-C31-O32	-2.03	118.56	123.63
86	3Q	501	HEC	CHB-C1B-C2B	-2.03	121.55	127.43
75	1H	401	CDL	OA8-CA7-OA9	-2.02	118.57	123.63
69	3C	503	3PE	O21-C21-O22	-2.02	118.98	123.70
69	3C	509	3PE	O21-C21-O22	-2.02	118.98	123.70
75	1i	201	CDL	OA6-CA5-OA7	-2.02	118.98	123.70
91	4A	609	PGV	O01-C1-O02	-2.02	118.98	123.70
75	4C	307	CDL	OB6-CB5-OB7	-2.02	118.98	123.70
69	1L	708	3PE	C3-C2-C1	-2.02	107.08	111.78
75	1i	201	CDL	OB6-CB5-OB7	-2.02	118.99	123.70
69	3C	503	3PE	O31-C31-O32	-2.02	118.59	123.63
75	3Y	106	CDL	OB6-CB5-OB7	-2.01	119.00	123.70
75	3P	513	CDL	OB8-CB7-OB9	-2.01	118.59	123.63
85	3C	502	HEM	C4D-ND-C1D	2.01	107.59	105.21
75	3N	502	CDL	OB8-CB7-OB9	-2.01	118.59	123.63
75	1N	402	CDL	OB6-CB5-OB7	-2.01	119.00	123.70
88	4A	602	HEA	CAD-CBD-CGD	-2.01	108.33	113.67
69	3P	510	3PE	O31-C31-O32	-2.01	118.60	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	3X	106	3PE	O31-C31-C32	2.01	117.96	111.83
77	1O	401	GTP	C5-C6-N1	2.01	118.36	113.25
69	3P	517	3PE	O31-C31-O32	-2.00	118.62	123.63
70	1h	203	PC1	O31-C31-O32	-2.00	118.62	123.63
85	3C	502	HEM	CHA-C1A-NA	2.00	127.49	123.86
69	1L	705	3PE	O31-C31-O32	-2.00	118.62	123.63
69	3X	101	3PE	C23-C22-C21	-2.00	106.35	113.69
69	1A	203	3PE	O21-C21-O22	-2.00	119.02	123.70
85	3P	501	HEM	CHA-C4D-C3D	-2.00	121.53	125.23
75	1q	202	CDL	CB4-OB6-CB5	-2.00	113.00	117.80
69	3P	519	3PE	C36-C35-C34	-2.00	104.25	114.37

There are no chirality outliers.

All (3142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	1A	201	3PE	C11-O13-P-O11
69	1A	201	3PE	C11-O13-P-O12
69	1A	201	3PE	C11-O13-P-O14
69	1A	203	3PE	C11-O13-P-O11
69	1A	203	3PE	C11-O13-P-O12
69	1A	203	3PE	C11-O13-P-O14
69	1B	204	3PE	C1-O11-P-O13
69	1B	204	3PE	C1-O11-P-O14
69	1B	205	3PE	C1-O11-P-O13
69	1B	205	3PE	C1-O11-P-O14
69	1B	205	3PE	C11-O13-P-O11
69	1B	205	3PE	C11-O13-P-O12
69	1B	205	3PE	C11-O13-P-O14
69	1B	205	3PE	C1-C2-O21-C21
69	1B	205	3PE	O22-C21-O21-C2
69	1B	205	3PE	C22-C21-O21-C2
69	1J	201	3PE	C1-O11-P-O13
69	1J	201	3PE	C1-O11-P-O14
69	1L	701	3PE	C11-O13-P-O11
69	1L	701	3PE	C11-O13-P-O12
69	1L	701	3PE	C11-O13-P-O14
69	1L	702	3PE	O22-C21-O21-C2
69	1L	702	3PE	C22-C21-O21-C2
69	1L	703	3PE	C1-O11-P-O12
69	1L	703	3PE	C11-O13-P-O11
69	1L	703	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	1L	703	3PE	C12-C11-O13-P
69	1L	705	3PE	C1-O11-P-O13
69	1L	705	3PE	C1-O11-P-O14
69	1L	706	3PE	C1-O11-P-O14
69	1L	706	3PE	C11-O13-P-O11
69	1L	707	3PE	O13-C11-C12-N
69	1L	708	3PE	C1-O11-P-O14
69	1L	708	3PE	O22-C21-O21-C2
69	1L	709	3PE	C1-O11-P-O12
69	1L	709	3PE	C1-O11-P-O13
69	1L	709	3PE	C11-O13-P-O11
69	1L	709	3PE	O22-C21-O21-C2
69	1L	709	3PE	C22-C21-O21-C2
69	1L	710	3PE	O22-C21-O21-C2
69	1L	711	3PE	O11-C1-C2-O21
69	1L	712	3PE	C1-O11-P-O13
69	1L	712	3PE	C11-O13-P-O11
69	1L	712	3PE	C11-O13-P-O12
69	1L	712	3PE	C11-O13-P-O14
69	1M	502	3PE	C1-O11-P-O13
69	1M	502	3PE	C11-O13-P-O14
69	1M	502	3PE	O11-C1-C2-O21
69	1M	502	3PE	C32-C31-O31-C3
69	1Y	201	3PE	C11-O13-P-O11
69	1Y	201	3PE	C11-O13-P-O12
69	1Y	201	3PE	C22-C21-O21-C2
69	1Y	204	3PE	C22-C21-O21-C2
69	1Y	205	3PE	C1-O11-P-O12
69	1Y	205	3PE	C1-O11-P-O13
69	1Y	205	3PE	C11-O13-P-O14
69	1Y	208	3PE	C11-O13-P-O11
69	1Y	208	3PE	C11-O13-P-O14
69	1Y	208	3PE	C12-C11-O13-P
69	1Y	209	3PE	C1-O11-P-O12
69	1Y	209	3PE	C1-O11-P-O13
69	1Y	209	3PE	C11-O13-P-O11
69	1Y	209	3PE	C11-O13-P-O12
69	1Y	209	3PE	C11-O13-P-O14
69	1Y	209	3PE	C22-C21-O21-C2
69	1Y	210	3PE	C1-O11-P-O13
69	1Y	210	3PE	C12-C11-O13-P
69	1Y	211	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	1Y	211	3PE	O22-C21-O21-C2
69	1Y	211	3PE	C22-C21-O21-C2
69	1Y	212	3PE	C1-O11-P-O14
69	1Y	212	3PE	C11-O13-P-O11
69	1Y	212	3PE	C11-O13-P-O12
69	1Y	212	3PE	C11-O13-P-O14
69	1Y	213	3PE	C1-O11-P-O13
69	1Y	213	3PE	C1-O11-P-O14
69	1Y	213	3PE	C11-O13-P-O11
69	1Y	213	3PE	O13-C11-C12-N
69	1Y	213	3PE	C32-C31-O31-C3
69	1Y	213	3PE	O22-C21-O21-C2
69	1Y	215	3PE	C1-O11-P-O13
69	1Y	215	3PE	C1-O11-P-O14
69	1Y	215	3PE	O32-C31-O31-C3
69	1Y	215	3PE	C32-C31-O31-C3
69	1Y	215	3PE	O22-C21-O21-C2
69	1Y	216	3PE	C1-O11-P-O12
69	1Y	216	3PE	C1-O11-P-O13
69	1Y	216	3PE	C1-O11-P-O14
69	1Y	216	3PE	C22-C21-O21-C2
69	1b	101	3PE	C11-O13-P-O11
69	1b	101	3PE	C22-C21-O21-C2
69	1d	201	3PE	C11-O13-P-O11
69	1d	201	3PE	C11-O13-P-O12
69	1d	201	3PE	O32-C31-O31-C3
69	1d	201	3PE	C32-C31-O31-C3
69	1d	203	3PE	C1-O11-P-O12
69	1d	203	3PE	C1-O11-P-O13
69	1d	203	3PE	C1-O11-P-O14
69	1d	203	3PE	O13-C11-C12-N
69	1d	203	3PE	O22-C21-O21-C2
69	1d	203	3PE	C22-C21-O21-C2
69	1d	206	3PE	C11-O13-P-O11
69	1d	206	3PE	C11-O13-P-O12
69	1e	201	3PE	C1-O11-P-O14
69	1e	201	3PE	C11-O13-P-O11
69	1e	201	3PE	C11-O13-P-O14
69	1f	101	3PE	C1-O11-P-O12
69	1f	101	3PE	C11-O13-P-O11
69	1f	101	3PE	C11-O13-P-O14
69	1f	102	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	1f	102	3PE	O13-C11-C12-N
69	1f	102	3PE	C22-C21-O21-C2
69	1f	103	3PE	C11-O13-P-O11
69	1f	103	3PE	C11-O13-P-O12
69	1f	103	3PE	C11-O13-P-O14
69	1f	103	3PE	O22-C21-O21-C2
69	1f	103	3PE	C22-C21-O21-C2
69	1f	104	3PE	C1-O11-P-O13
69	1f	104	3PE	C11-O13-P-O12
69	1f	104	3PE	C11-O13-P-O14
69	1g	202	3PE	C11-O13-P-O12
69	1g	202	3PE	C12-C11-O13-P
69	1g	202	3PE	C22-C21-O21-C2
69	1g	203	3PE	C1-O11-P-O12
69	1g	203	3PE	C1-O11-P-O13
69	1h	204	3PE	C1-O11-P-O12
69	1h	204	3PE	C1-O11-P-O13
69	1h	204	3PE	C1-O11-P-O14
69	1h	204	3PE	C11-O13-P-O11
69	1h	204	3PE	C11-O13-P-O12
69	1h	204	3PE	C11-O13-P-O14
69	1h	204	3PE	O22-C21-O21-C2
69	1k	101	3PE	C1-O11-P-O13
69	1k	101	3PE	O21-C2-C3-O31
69	1k	101	3PE	O22-C21-O21-C2
69	1l	202	3PE	C11-O13-P-O11
69	1l	202	3PE	C11-O13-P-O12
69	1l	203	3PE	C11-O13-P-O11
69	1l	203	3PE	C11-O13-P-O14
69	1l	203	3PE	C22-C21-O21-C2
69	1l	204	3PE	C11-O13-P-O11
69	1l	204	3PE	C11-O13-P-O12
69	1l	204	3PE	C11-O13-P-O14
69	1l	204	3PE	O22-C21-O21-C2
69	1m	201	3PE	C1-O11-P-O13
69	1m	202	3PE	C22-C21-O21-C2
69	1m	203	3PE	C1-O11-P-O12
69	1m	203	3PE	C1-O11-P-O13
69	1m	203	3PE	C1-O11-P-O14
69	1m	203	3PE	C11-O13-P-O11
69	1m	203	3PE	O22-C21-O21-C2
69	1m	203	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	1m	204	3PE	C1-O11-P-O12
69	1m	205	3PE	C11-O13-P-O11
69	1m	205	3PE	C11-O13-P-O12
69	1m	205	3PE	C22-C21-O21-C2
69	1o	201	3PE	C1-O11-P-O12
69	1o	201	3PE	C1-O11-P-O13
69	1o	201	3PE	C1-O11-P-O14
69	1o	201	3PE	C11-O13-P-O11
69	1o	201	3PE	C11-O13-P-O12
69	1o	201	3PE	C11-O13-P-O14
69	3A	502	3PE	C1-O11-P-O12
69	3A	502	3PE	C11-O13-P-O11
69	3A	502	3PE	C11-O13-P-O12
69	3A	502	3PE	O22-C21-O21-C2
69	3A	502	3PE	C22-C21-O21-C2
69	3A	503	3PE	C1-O11-P-O13
69	3A	503	3PE	C1-O11-P-O14
69	3A	503	3PE	C11-O13-P-O11
69	3A	503	3PE	C11-O13-P-O12
69	3A	503	3PE	C12-C11-O13-P
69	3A	503	3PE	O22-C21-O21-C2
69	3A	503	3PE	C22-C21-O21-C2
69	3C	503	3PE	C11-O13-P-O12
69	3C	505	3PE	C1-O11-P-O13
69	3C	506	3PE	C1-O11-P-O14
69	3C	507	3PE	C1-O11-P-O12
69	3C	507	3PE	C1-O11-P-O13
69	3C	507	3PE	C1-O11-P-O14
69	3C	507	3PE	C11-O13-P-O11
69	3C	507	3PE	C11-O13-P-O12
69	3C	507	3PE	C11-O13-P-O14
69	3C	507	3PE	C22-C21-O21-C2
69	3C	508	3PE	C11-O13-P-O14
69	3C	508	3PE	O22-C21-O21-C2
69	3C	509	3PE	C1-O11-P-O12
69	3C	509	3PE	C1-O11-P-O13
69	3C	509	3PE	C11-O13-P-O14
69	3C	510	3PE	C1-O11-P-O14
69	3C	510	3PE	C11-O13-P-O14
69	3C	510	3PE	O21-C2-C3-O31
69	3C	511	3PE	C1-O11-P-O13
69	3C	511	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	3C	511	3PE	C22-C21-O21-C2
69	3C	512	3PE	O13-C11-C12-N
69	3C	512	3PE	O22-C21-O21-C2
69	3C	513	3PE	C1-O11-P-O12
69	3C	513	3PE	C1-O11-P-O13
69	3C	513	3PE	C22-C21-O21-C2
69	3C	514	3PE	C1-O11-P-O13
69	3C	515	3PE	C1-O11-P-O12
69	3C	515	3PE	C1-O11-P-O13
69	3C	515	3PE	C1-O11-P-O14
69	3C	515	3PE	C11-O13-P-O14
69	3C	515	3PE	C22-C21-O21-C2
69	3C	516	3PE	C11-O13-P-O11
69	3C	516	3PE	C11-O13-P-O14
69	3C	516	3PE	C1-C2-O21-C21
69	3C	516	3PE	O22-C21-O21-C2
69	3C	516	3PE	C22-C21-O21-C2
69	3D	502	3PE	C1-O11-P-O13
69	3D	502	3PE	C2-C1-O11-P
69	3D	502	3PE	C22-C21-O21-C2
69	3D	503	3PE	C11-O13-P-O11
69	3D	503	3PE	C11-O13-P-O12
69	3D	503	3PE	O13-C11-C12-N
69	3D	503	3PE	C22-C21-O21-C2
69	3E	302	3PE	C1-O11-P-O12
69	3E	302	3PE	C1-O11-P-O13
69	3E	302	3PE	C11-O13-P-O11
69	3E	302	3PE	C11-O13-P-O12
69	3E	302	3PE	C11-O13-P-O14
69	3E	303	3PE	C1-O11-P-O14
69	3G	101	3PE	C11-O13-P-O14
69	3G	102	3PE	C1-O11-P-O13
69	3G	102	3PE	C11-O13-P-O12
69	3G	103	3PE	C11-O13-P-O11
69	3G	103	3PE	C11-O13-P-O12
69	3G	103	3PE	C11-O13-P-O14
69	3G	103	3PE	C22-C21-O21-C2
69	3G	104	3PE	C1-O11-P-O13
69	3G	104	3PE	C1-O11-P-O14
69	3G	104	3PE	C11-O13-P-O11
69	3G	104	3PE	C11-O13-P-O12
69	3G	104	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
69	3G	104	3PE	O22-C21-O21-C2
69	3G	104	3PE	C22-C21-O21-C2
69	3G	105	3PE	C1-O11-P-O12
69	3G	105	3PE	C1-O11-P-O13
69	3G	105	3PE	C1-O11-P-O14
69	3G	105	3PE	C11-O13-P-O11
69	3G	105	3PE	C11-O13-P-O12
69	3G	105	3PE	C11-O13-P-O14
69	3G	105	3PE	C22-C21-O21-C2
69	3G	106	3PE	C1-O11-P-O13
69	3G	106	3PE	C1-O11-P-O14
69	3G	106	3PE	C2-C3-O31-C31
69	3G	106	3PE	O22-C21-O21-C2
69	3G	106	3PE	C22-C21-O21-C2
69	3G	108	3PE	C1-O11-P-O13
69	3G	108	3PE	C1-O11-P-O14
69	3G	108	3PE	O11-C1-C2-O21
69	3G	108	3PE	C22-C21-O21-C2
69	3G	109	3PE	C1-O11-P-O12
69	3G	109	3PE	C1-O11-P-O13
69	3G	109	3PE	C11-O13-P-O14
69	3G	109	3PE	C2-C1-O11-P
69	3G	110	3PE	C1-O11-P-O14
69	3G	110	3PE	C22-C21-O21-C2
69	3G	111	3PE	C1-O11-P-O12
69	3G	111	3PE	C1-O11-P-O13
69	3G	111	3PE	C11-O13-P-O12
69	3G	111	3PE	C11-O13-P-O14
69	3G	111	3PE	C22-C21-O21-C2
69	3J	101	3PE	C1-O11-P-O12
69	3J	101	3PE	C1-O11-P-O13
69	3J	101	3PE	C1-O11-P-O14
69	3J	101	3PE	C11-O13-P-O11
69	3J	101	3PE	C2-C3-O31-C31
69	3J	101	3PE	O22-C21-O21-C2
69	3J	102	3PE	C1-O11-P-O13
69	3J	102	3PE	C11-O13-P-O11
69	3J	102	3PE	C11-O13-P-O12
69	3J	103	3PE	C1-O11-P-O13
69	3J	103	3PE	C1-O11-P-O14
69	3J	103	3PE	C11-O13-P-O11
69	3J	103	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	3J	104	3PE	C1-O11-P-O13
69	3J	104	3PE	C1-O11-P-O14
69	3J	104	3PE	C22-C21-O21-C2
69	3J	105	3PE	C11-O13-P-O14
69	3J	105	3PE	C22-C21-O21-C2
69	3N	501	3PE	C1-O11-P-O14
69	3N	501	3PE	C11-O13-P-O14
69	3N	501	3PE	O13-C11-C12-N
69	3N	501	3PE	C22-C21-O21-C2
69	3N	503	3PE	C1-O11-P-O14
69	3N	503	3PE	C11-O13-P-O11
69	3N	503	3PE	C11-O13-P-O12
69	3N	503	3PE	O22-C21-O21-C2
69	3N	503	3PE	C22-C21-O21-C2
69	3P	503	3PE	C1-O11-P-O13
69	3P	503	3PE	C1-O11-P-O14
69	3P	503	3PE	C22-C21-O21-C2
69	3P	504	3PE	C11-O13-P-O11
69	3P	504	3PE	C22-C21-O21-C2
69	3P	505	3PE	O22-C21-O21-C2
69	3P	505	3PE	C22-C21-O21-C2
69	3P	506	3PE	C1-O11-P-O12
69	3P	506	3PE	C1-O11-P-O13
69	3P	506	3PE	C12-C11-O13-P
69	3P	506	3PE	O22-C21-O21-C2
69	3P	507	3PE	C1-O11-P-O14
69	3P	507	3PE	C11-O13-P-O11
69	3P	507	3PE	C11-O13-P-O12
69	3P	508	3PE	C11-O13-P-O11
69	3P	508	3PE	O13-C11-C12-N
69	3P	510	3PE	C1-O11-P-O13
69	3P	510	3PE	C1-O11-P-O14
69	3P	512	3PE	C11-O13-P-O11
69	3P	512	3PE	C11-O13-P-O12
69	3P	512	3PE	C11-O13-P-O14
69	3P	514	3PE	C11-O13-P-O11
69	3P	514	3PE	C11-O13-P-O12
69	3P	514	3PE	C11-O13-P-O14
69	3P	514	3PE	C22-C21-O21-C2
69	3P	515	3PE	C1-O11-P-O13
69	3P	515	3PE	C1-O11-P-O14
69	3P	515	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
69	3P	515	3PE	C11-O13-P-O12
69	3P	515	3PE	C11-O13-P-O14
69	3P	515	3PE	C12-C11-O13-P
69	3P	515	3PE	C3-C2-O21-C21
69	3P	515	3PE	O22-C21-O21-C2
69	3P	515	3PE	C22-C21-O21-C2
69	3P	516	3PE	C1-O11-P-O12
69	3P	516	3PE	C1-O11-P-O13
69	3P	516	3PE	C11-O13-P-O14
69	3P	517	3PE	C1-O11-P-O13
69	3P	517	3PE	C1-O11-P-O14
69	3P	517	3PE	C2-C1-O11-P
69	3P	518	3PE	C1-O11-P-O12
69	3P	518	3PE	C1-O11-P-O13
69	3P	518	3PE	C1-O11-P-O14
69	3P	518	3PE	C11-O13-P-O11
69	3P	518	3PE	C11-O13-P-O12
69	3P	518	3PE	O22-C21-O21-C2
69	3P	518	3PE	C22-C21-O21-C2
69	3P	519	3PE	C11-O13-P-O11
69	3P	519	3PE	C11-O13-P-O12
69	3P	519	3PE	C11-O13-P-O14
69	3P	520	3PE	C1-O11-P-O14
69	3P	520	3PE	O22-C21-O21-C2
69	3Q	502	3PE	O22-C21-O21-C2
69	3Q	503	3PE	C2-C3-O31-C31
69	3Q	503	3PE	C22-C21-O21-C2
69	3Q	504	3PE	C22-C21-O21-C2
69	3R	302	3PE	C1-O11-P-O12
69	3R	302	3PE	C11-O13-P-O11
69	3R	302	3PE	C11-O13-P-O12
69	3R	302	3PE	C11-O13-P-O14
69	3R	304	3PE	C11-O13-P-O11
69	3R	304	3PE	C11-O13-P-O12
69	3R	304	3PE	C11-O13-P-O14
69	3R	305	3PE	C11-O13-P-O14
69	3R	305	3PE	C12-C11-O13-P
69	3R	305	3PE	O32-C31-O31-C3
69	3R	305	3PE	C32-C31-O31-C3
69	3R	305	3PE	O22-C21-O21-C2
69	3S	201	3PE	C1-O11-P-O12
69	3S	201	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
69	3S	201	3PE	C11-O13-P-O12
69	3S	201	3PE	C22-C21-O21-C2
69	3T	103	3PE	C1-O11-P-O13
69	3T	103	3PE	C11-O13-P-O11
69	3W	101	3PE	C1-O11-P-O12
69	3W	101	3PE	C1-O11-P-O13
69	3W	101	3PE	C1-O11-P-O14
69	3W	101	3PE	O13-C11-C12-N
69	3W	101	3PE	C22-C21-O21-C2
69	3W	102	3PE	C1-O11-P-O12
69	3W	102	3PE	C1-O11-P-O14
69	3W	102	3PE	C11-O13-P-O11
69	3W	102	3PE	C11-O13-P-O14
69	3W	102	3PE	O32-C31-O31-C3
69	3W	102	3PE	C32-C31-O31-C3
69	3W	103	3PE	C22-C21-O21-C2
69	3X	101	3PE	C1-O11-P-O13
69	3X	101	3PE	C1-O11-P-O14
69	3X	105	3PE	C1-O11-P-O12
69	3X	105	3PE	C1-O11-P-O13
69	3X	105	3PE	C1-O11-P-O14
69	3X	106	3PE	C1-O11-P-O13
69	3X	106	3PE	C1-O11-P-O14
69	3X	106	3PE	O32-C31-O31-C3
69	3X	106	3PE	C32-C31-O31-C3
69	3X	106	3PE	C22-C21-O21-C2
69	3X	107	3PE	C1-O11-P-O13
69	3X	107	3PE	C11-O13-P-O11
69	3X	107	3PE	C11-O13-P-O12
69	3X	107	3PE	C11-O13-P-O14
69	3Y	101	3PE	C1-O11-P-O12
69	3Y	101	3PE	C1-O11-P-O13
69	3Y	101	3PE	C1-O11-P-O14
69	3Y	101	3PE	C11-O13-P-O11
69	3Y	101	3PE	C11-O13-P-O12
69	3Y	101	3PE	C11-O13-P-O14
69	3Y	102	3PE	C1-O11-P-O12
69	3Y	102	3PE	C1-O11-P-O13
69	3Y	102	3PE	O32-C31-O31-C3
69	3Y	104	3PE	C1-O11-P-O14
69	3Y	107	3PE	C1-O11-P-O14
69	3Y	107	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
69	3Y	107	3PE	C22-C21-O21-C2
69	4G	101	3PE	C1-O11-P-O14
69	4G	101	3PE	C11-O13-P-O11
69	4G	101	3PE	C2-C3-O31-C31
69	4G	101	3PE	C22-C21-O21-C2
70	1A	202	PC1	C1-O11-P-O12
70	1A	202	PC1	C1-O11-P-O13
70	1A	202	PC1	O22-C21-O21-C2
70	1B	202	PC1	C11-O13-P-O12
70	1B	202	PC1	C11-O13-P-O11
70	1B	202	PC1	C1-O11-P-O14
70	1B	202	PC1	C1-O11-P-O13
70	1B	203	PC1	C11-O13-P-O14
70	1B	203	PC1	C11-O13-P-O11
70	1B	203	PC1	C1-O11-P-O12
70	1B	203	PC1	C1-O11-P-O14
70	1B	203	PC1	C1-O11-P-O13
70	1H	402	PC1	C11-O13-P-O14
70	1J	202	PC1	C11-O13-P-O14
70	1J	202	PC1	C1-O11-P-O14
70	1M	501	PC1	C11-O13-P-O14
70	1M	501	PC1	C11-O13-P-O11
70	1M	501	PC1	C1-O11-P-O12
70	1M	501	PC1	C1-O11-P-O14
70	1P	502	PC1	C1-O11-P-O12
70	1P	502	PC1	C1-O11-P-O14
70	1P	502	PC1	C1-O11-P-O13
70	1P	502	PC1	O13-C11-C12-N
70	1Y	202	PC1	C11-O13-P-O12
70	1Y	202	PC1	C11-O13-P-O14
70	1Y	202	PC1	C1-O11-P-O12
70	1Y	202	PC1	C1-O11-P-O14
70	1Y	202	PC1	C1-O11-P-O13
70	1Y	202	PC1	C22-C21-O21-C2
70	1Y	206	PC1	C11-O13-P-O11
70	1Y	206	PC1	C1-O11-P-O12
70	1Y	206	PC1	C1-O11-P-O13
70	1Y	207	PC1	C11-O13-P-O12
70	1Y	207	PC1	C11-O13-P-O14
70	1Y	207	PC1	C11-O13-P-O11
70	1Y	207	PC1	O32-C31-O31-C3
70	1Y	207	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
70	1d	204	PC1	C11-O13-P-O12
70	1d	204	PC1	C11-O13-P-O11
70	1d	204	PC1	C1-O11-P-O14
70	1d	204	PC1	C1-O11-P-O13
70	1d	204	PC1	C12-C11-O13-P
70	1d	204	PC1	O13-C11-C12-N
70	1d	204	PC1	C2-C1-O11-P
70	1d	204	PC1	C22-C21-O21-C2
70	1d	204	PC1	O32-C31-O31-C3
70	1d	204	PC1	C32-C31-O31-C3
70	1h	203	PC1	C11-O13-P-O11
70	1h	203	PC1	C1-O11-P-O12
70	1h	203	PC1	C1-O11-P-O14
70	1h	203	PC1	C1-O11-P-O13
70	3J	106	PC1	C1-O11-P-O14
70	3J	106	PC1	C1-O11-P-O13
70	3P	509	PC1	C11-O13-P-O11
70	3P	509	PC1	O13-C11-C12-N
70	3R	303	PC1	C11-O13-P-O12
70	3R	303	PC1	C11-O13-P-O11
70	3T	102	PC1	C11-O13-P-O11
70	3T	102	PC1	C1-O11-P-O13
70	3T	102	PC1	C22-C21-O21-C2
70	3X	104	PC1	C11-O13-P-O12
75	1H	401	CDL	CA2-OA2-PA1-OA3
75	1H	401	CDL	CA2-OA2-PA1-OA5
75	1H	401	CDL	CA3-OA5-PA1-OA4
75	1H	401	CDL	CB2-OB2-PB2-OB3
75	1H	401	CDL	CB2-OB2-PB2-OB5
75	1H	401	CDL	CB3-OB5-PB2-OB2
75	1H	401	CDL	CB3-OB5-PB2-OB3
75	1H	401	CDL	CB3-OB5-PB2-OB4
75	1H	401	CDL	OB7-CB5-OB6-CB4
75	1H	401	CDL	C51-CB5-OB6-CB4
75	1L	704	CDL	CA2-OA2-PA1-OA5
75	1L	704	CDL	CB3-OB5-PB2-OB2
75	1L	704	CDL	CB3-OB5-PB2-OB3
75	1L	704	CDL	OB7-CB5-OB6-CB4
75	1N	402	CDL	CA2-OA2-PA1-OA4
75	1N	402	CDL	CA2-OA2-PA1-OA5
75	1N	402	CDL	CA3-OA5-PA1-OA2
75	1N	402	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	1N	402	CDL	CB2-OB2-PB2-OB4
75	1Y	217	CDL	C1-CA2-OA2-PA1
75	1Y	217	CDL	CA2-OA2-PA1-OA4
75	1Y	217	CDL	CA2-OA2-PA1-OA5
75	1Y	217	CDL	CA3-OA5-PA1-OA3
75	1Y	217	CDL	C1-CB2-OB2-PB2
75	1Y	217	CDL	CB3-OB5-PB2-OB3
75	1d	202	CDL	CA3-OA5-PA1-OA2
75	1d	202	CDL	CB2-OB2-PB2-OB3
75	1d	202	CDL	CB2-OB2-PB2-OB5
75	1d	202	CDL	OB7-CB5-OB6-CB4
75	1d	202	CDL	C51-CB5-OB6-CB4
75	1d	205	CDL	CA3-OA5-PA1-OA2
75	1d	205	CDL	CA3-OA5-PA1-OA3
75	1d	205	CDL	CB3-OB5-PB2-OB3
75	1g	201	CDL	CA2-OA2-PA1-OA3
75	1g	201	CDL	CA2-OA2-PA1-OA4
75	1g	201	CDL	CA2-OA2-PA1-OA5
75	1g	201	CDL	CA3-OA5-PA1-OA2
75	1g	201	CDL	CA3-OA5-PA1-OA3
75	1g	201	CDL	CB2-OB2-PB2-OB4
75	1g	201	CDL	CB2-OB2-PB2-OB5
75	1g	201	CDL	C51-CB5-OB6-CB4
75	1i	201	CDL	CA2-OA2-PA1-OA4
75	1i	201	CDL	CA2-OA2-PA1-OA5
75	1i	201	CDL	OB7-CB5-OB6-CB4
75	1q	201	CDL	CA2-OA2-PA1-OA4
75	1q	201	CDL	CA3-OA5-PA1-OA3
75	1q	201	CDL	C11-CA5-OA6-CA4
75	1q	202	CDL	CB2-OB2-PB2-OB3
75	1q	202	CDL	CB3-OB5-PB2-OB2
75	1q	202	CDL	CB3-OB5-PB2-OB3
75	1q	202	CDL	CB3-OB5-PB2-OB4
75	1q	202	CDL	OB6-CB4-CB6-OB8
75	3A	501	CDL	CA2-OA2-PA1-OA3
75	3A	501	CDL	CA2-OA2-PA1-OA5
75	3A	501	CDL	CB2-OB2-PB2-OB3
75	3A	501	CDL	CB2-OB2-PB2-OB5
75	3A	501	CDL	CB3-OB5-PB2-OB3
75	3A	501	CDL	OB7-CB5-OB6-CB4
75	3D	504	CDL	CA2-OA2-PA1-OA4
75	3D	504	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
75	3D	504	CDL	C11-CA5-OA6-CA4
75	3D	504	CDL	CB2-OB2-PB2-OB3
75	3D	504	CDL	CB2-OB2-PB2-OB5
75	3F	201	CDL	CA2-OA2-PA1-OA4
75	3F	201	CDL	CA2-OA2-PA1-OA5
75	3F	201	CDL	CA3-OA5-PA1-OA2
75	3F	201	CDL	CA3-OA5-PA1-OA3
75	3F	201	CDL	CA3-OA5-PA1-OA4
75	3F	201	CDL	CB2-OB2-PB2-OB5
75	3F	201	CDL	CB3-OB5-PB2-OB2
75	3F	201	CDL	CB3-OB5-PB2-OB3
75	3F	201	CDL	CB3-OB5-PB2-OB4
75	3F	201	CDL	OB7-CB5-OB6-CB4
75	3F	201	CDL	C51-CB5-OB6-CB4
75	3N	502	CDL	CA3-OA5-PA1-OA2
75	3N	502	CDL	CA3-OA5-PA1-OA4
75	3N	502	CDL	C11-CA5-OA6-CA4
75	3N	502	CDL	CB2-OB2-PB2-OB3
75	3N	502	CDL	CB2-OB2-PB2-OB4
75	3N	502	CDL	CB3-OB5-PB2-OB2
75	3N	502	CDL	C51-CB5-OB6-CB4
75	3P	513	CDL	CA2-OA2-PA1-OA4
75	3P	513	CDL	CA2-OA2-PA1-OA5
75	3T	101	CDL	CA2-OA2-PA1-OA3
75	3T	101	CDL	CA2-OA2-PA1-OA4
75	3T	101	CDL	CA2-OA2-PA1-OA5
75	3T	101	CDL	CB3-OB5-PB2-OB2
75	3T	101	CDL	CB3-OB5-PB2-OB3
75	3T	101	CDL	CB3-OB5-PB2-OB4
75	3T	101	CDL	OB6-CB4-CB6-OB8
75	3X	103	CDL	CA3-OA5-PA1-OA2
75	3X	103	CDL	CA3-OA5-PA1-OA3
75	3X	103	CDL	C11-CA5-OA6-CA4
75	3X	103	CDL	CB2-OB2-PB2-OB3
75	3X	103	CDL	CB2-OB2-PB2-OB4
75	3X	103	CDL	CB2-OB2-PB2-OB5
75	3X	103	CDL	CB3-OB5-PB2-OB3
75	3X	103	CDL	CB3-OB5-PB2-OB4
75	3X	103	CDL	CB4-CB3-OB5-PB2
75	3X	103	CDL	C51-CB5-OB6-CB4
75	3Y	106	CDL	O1-C1-CA2-OA2
75	3Y	106	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
75	3Y	106	CDL	CA2-OA2-PA1-OA5
75	3Y	106	CDL	CA3-OA5-PA1-OA3
75	3Y	106	CDL	CA3-OA5-PA1-OA4
75	3Y	106	CDL	CB2-OB2-PB2-OB3
75	3Y	106	CDL	CB3-OB5-PB2-OB2
75	3Y	106	CDL	CB3-OB5-PB2-OB4
75	3Y	106	CDL	OB7-CB5-OB6-CB4
75	3Y	106	CDL	C51-CB5-OB6-CB4
75	4B	302	CDL	CB2-OB2-PB2-OB5
75	4B	302	CDL	CB3-OB5-PB2-OB2
75	4B	302	CDL	CB3-OB5-PB2-OB3
75	4B	302	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	CA3-OA5-PA1-OA2
75	4C	306	CDL	CA3-OA5-PA1-OA3
75	4C	306	CDL	CA3-OA5-PA1-OA4
75	4C	306	CDL	C11-CA5-OA6-CA4
75	4C	306	CDL	CB2-OB2-PB2-OB3
75	4C	306	CDL	CB3-OB5-PB2-OB2
75	4C	306	CDL	CB3-OB5-PB2-OB3
75	4C	306	CDL	CB3-OB5-PB2-OB4
75	4C	306	CDL	OB7-CB5-OB6-CB4
75	4C	307	CDL	CA3-OA5-PA1-OA2
75	4C	307	CDL	CA3-OA5-PA1-OA3
75	4C	307	CDL	CA3-OA5-PA1-OA4
75	4C	307	CDL	CB2-OB2-PB2-OB5
75	4C	307	CDL	CB3-OB5-PB2-OB2
75	4C	307	CDL	CB3-OB5-PB2-OB4
81	1T	101	EHZ	N2-C15-C16-O5
82	1Y	203	PGT	C32-C31-O2-C2
82	1Y	203	PGT	O31-C31-O2-C2
82	1Y	203	PGT	C1-O3P-P-O2P
82	1Y	203	PGT	C4-O4P-P-O2P
82	1Y	203	PGT	O11-C11-O3-C3
82	1Y	203	PGT	C12-C11-O3-C3
84	1l	201	MYR	O1-C1-C2-C3
85	3C	501	HEM	C2B-C3B-CAB-CBB
85	3C	502	HEM	C2B-C3B-CAB-CBB
85	3P	502	HEM	C2B-C3B-CAB-CBB
85	3P	502	HEM	C2C-C3C-CAC-CBC
85	3P	502	HEM	C4C-C3C-CAC-CBC
87	3X	102	PEK	C03-O11-P-O14
87	3X	102	PEK	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
87	3X	102	PEK	C11-C10-C9-C8
87	4G	103	PEK	C04-O12-P-O11
87	4G	103	PEK	C04-O12-P-O14
88	4A	601	HEA	C3B-C11-C12-C13
88	4A	602	HEA	C2A-C3A-CMA-OMA
88	4A	602	HEA	C4A-C3A-CMA-OMA
91	4A	606	PGV	C03-O11-P-O12
91	4A	606	PGV	C01-C02-O01-C1
91	4A	606	PGV	C2-C1-O01-C02
91	4A	607	PGV	C03-O11-P-O13
91	4A	607	PGV	C04-O12-P-O11
91	4A	607	PGV	C04-O12-P-O13
91	4A	608	PGV	C03-O11-P-O12
91	4A	608	PGV	C03-O11-P-O14
91	4A	609	PGV	C04-O12-P-O11
91	4C	302	PGV	C03-O11-P-O12
91	4C	302	PGV	C03-O11-P-O14
91	4C	302	PGV	C04-O12-P-O13
91	4C	303	PGV	C04-O12-P-O11
91	4C	304	PGV	O02-C1-O01-C02
91	4C	305	PGV	C03-O11-P-O12
91	4C	305	PGV	C04-O12-P-O11
91	4C	305	PGV	C04-O12-P-O13
91	4C	305	PGV	C04-O12-P-O14
91	4G	102	PGV	C03-O11-P-O12
91	4G	102	PGV	C03-O11-P-O13
91	4G	102	PGV	C03-O11-P-O14
91	4G	102	PGV	C04-O12-P-O13
91	4G	102	PGV	C04-O12-P-O14
91	4J	101	PGV	C03-O11-P-O12
91	4J	101	PGV	C03-O11-P-O13
91	4K	101	PGV	C03-O11-P-O12
91	4K	101	PGV	C03-O11-P-O13
91	4N	101	PGV	C03-O11-P-O13
91	4N	101	PGV	C04-O12-P-O11
91	4N	101	PGV	C04-O12-P-O13
91	4N	101	PGV	C04-O12-P-O14
93	4B	303	PSC	C03-O11-P-O13
93	4B	303	PSC	C03-O11-P-O14
93	4B	303	PSC	C04-O12-P-O14
93	4B	303	PSC	O12-C04-C05-N
93	4B	303	PSC	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
93	4B	303	PSC	C2-C1-O01-C02
69	1B	205	3PE	O32-C31-O31-C3
69	1M	502	3PE	O32-C31-O31-C3
69	1Y	213	3PE	O32-C31-O31-C3
69	1l	203	3PE	O32-C31-O31-C3
69	3C	513	3PE	O32-C31-O31-C3
69	3P	511	3PE	O32-C31-O31-C3
69	3Y	107	3PE	O32-C31-O31-C3
70	1J	202	PC1	O32-C31-O31-C3
75	3N	502	CDL	OB9-CB7-OB8-CB6
75	4B	302	CDL	OB9-CB7-OB8-CB6
69	3P	507	3PE	C2-C3-O31-C31
70	1Y	202	PC1	C2-C3-O31-C31
75	1H	401	CDL	CB4-CB6-OB8-CB7
69	1l	203	3PE	C32-C31-O31-C3
69	3C	513	3PE	C32-C31-O31-C3
69	3P	511	3PE	C32-C31-O31-C3
70	1J	202	PC1	C32-C31-O31-C3
75	3N	502	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	C71-CB7-OB8-CB6
69	1L	701	3PE	O32-C31-O31-C3
69	1Y	201	3PE	O32-C31-O31-C3
69	1b	101	3PE	O32-C31-O31-C3
69	1l	204	3PE	O32-C31-O31-C3
69	1m	204	3PE	O32-C31-O31-C3
69	3C	503	3PE	O32-C31-O31-C3
69	3C	506	3PE	O32-C31-O31-C3
69	3D	502	3PE	O32-C31-O31-C3
69	3G	106	3PE	O32-C31-O31-C3
69	3N	501	3PE	O32-C31-O31-C3
69	3W	103	3PE	O32-C31-O31-C3
69	3X	101	3PE	O32-C31-O31-C3
69	4G	104	3PE	O32-C31-O31-C3
75	1d	205	CDL	OA9-CA7-OA8-CA6
75	3T	101	CDL	OB9-CB7-OB8-CB6
75	4B	302	CDL	OA9-CA7-OA8-CA6
75	4C	306	CDL	OB9-CB7-OB8-CB6
91	4A	606	PGV	O04-C19-O03-C01
69	1Y	201	3PE	O22-C21-O21-C2
69	1Y	204	3PE	O22-C21-O21-C2
69	1Y	216	3PE	O22-C21-O21-C2
69	1b	101	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
69	1d	201	3PE	O22-C21-O21-C2
69	1f	102	3PE	O22-C21-O21-C2
69	1g	202	3PE	O22-C21-O21-C2
69	1l	203	3PE	O22-C21-O21-C2
69	1m	205	3PE	O22-C21-O21-C2
69	3C	507	3PE	O22-C21-O21-C2
69	3C	513	3PE	O22-C21-O21-C2
69	3C	515	3PE	O22-C21-O21-C2
69	3D	502	3PE	O22-C21-O21-C2
69	3D	503	3PE	O22-C21-O21-C2
69	3G	103	3PE	O22-C21-O21-C2
69	3G	105	3PE	O22-C21-O21-C2
69	3G	108	3PE	O22-C21-O21-C2
69	3G	110	3PE	O22-C21-O21-C2
69	3G	111	3PE	O22-C21-O21-C2
69	3J	104	3PE	O22-C21-O21-C2
69	3J	105	3PE	O22-C21-O21-C2
69	3P	504	3PE	O22-C21-O21-C2
69	3P	514	3PE	O22-C21-O21-C2
69	3Q	503	3PE	O22-C21-O21-C2
69	3Q	504	3PE	O22-C21-O21-C2
69	3S	201	3PE	O22-C21-O21-C2
69	3W	101	3PE	O22-C21-O21-C2
69	3W	103	3PE	O22-C21-O21-C2
69	3X	106	3PE	O22-C21-O21-C2
69	3Y	107	3PE	O22-C21-O21-C2
69	4G	101	3PE	O22-C21-O21-C2
70	1Y	202	PC1	O22-C21-O21-C2
70	3T	102	PC1	O22-C21-O21-C2
75	1H	401	CDL	OA7-CA5-OA6-CA4
75	1g	201	CDL	OB7-CB5-OB6-CB4
75	1q	201	CDL	OA7-CA5-OA6-CA4
75	3D	504	CDL	OA7-CA5-OA6-CA4
75	3N	502	CDL	OA7-CA5-OA6-CA4
75	3N	502	CDL	OB7-CB5-OB6-CB4
75	3X	103	CDL	OA7-CA5-OA6-CA4
75	3X	103	CDL	OB7-CB5-OB6-CB4
75	3Y	106	CDL	OA7-CA5-OA6-CA4
75	4C	306	CDL	OA7-CA5-OA6-CA4
91	4A	606	PGV	O02-C1-O01-C02
69	1h	204	3PE	C2-C3-O31-C31
69	1B	205	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	1L	701	3PE	C32-C31-O31-C3
69	1Y	201	3PE	C32-C31-O31-C3
69	1k	101	3PE	C32-C31-O31-C3
69	1l	204	3PE	C32-C31-O31-C3
69	1m	204	3PE	C32-C31-O31-C3
69	3C	506	3PE	C32-C31-O31-C3
69	3D	502	3PE	C32-C31-O31-C3
69	3G	106	3PE	C32-C31-O31-C3
69	3N	501	3PE	C32-C31-O31-C3
69	3R	304	3PE	C32-C31-O31-C3
69	3X	101	3PE	C32-C31-O31-C3
69	3Y	102	3PE	C32-C31-O31-C3
69	3Y	107	3PE	C32-C31-O31-C3
69	4G	104	3PE	C32-C31-O31-C3
75	1Y	217	CDL	C71-CB7-OB8-CB6
75	3T	101	CDL	C31-CA7-OA8-CA6
75	3T	101	CDL	C71-CB7-OB8-CB6
75	4B	302	CDL	C31-CA7-OA8-CA6
75	4C	306	CDL	C71-CB7-OB8-CB6
69	1L	708	3PE	C22-C21-O21-C2
69	1Y	213	3PE	C22-C21-O21-C2
69	1Y	215	3PE	C22-C21-O21-C2
69	1h	204	3PE	C22-C21-O21-C2
69	1k	101	3PE	C22-C21-O21-C2
69	1l	204	3PE	C22-C21-O21-C2
69	3C	508	3PE	C22-C21-O21-C2
69	3C	512	3PE	C22-C21-O21-C2
69	3J	101	3PE	C22-C21-O21-C2
69	3P	506	3PE	C22-C21-O21-C2
69	3P	520	3PE	C22-C21-O21-C2
69	3R	305	3PE	C22-C21-O21-C2
70	1A	202	PC1	C22-C21-O21-C2
75	1H	401	CDL	C11-CA5-OA6-CA4
75	1L	704	CDL	C51-CB5-OB6-CB4
75	1i	201	CDL	C51-CB5-OB6-CB4
75	3A	501	CDL	C51-CB5-OB6-CB4
75	3Y	106	CDL	C11-CA5-OA6-CA4
75	4C	306	CDL	C51-CB5-OB6-CB4
91	4C	304	PGV	C2-C1-O01-C02
69	3C	507	3PE	O32-C31-O31-C3
70	1M	501	PC1	O32-C31-O31-C3
81	1T	101	EHZ	C13-C12-N1-C11

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Mol	Chain	Res	Type	Atoms
69	1o	201	3PE	O32-C31-O31-C3
69	3C	514	3PE	O32-C31-O31-C3
75	3T	101	CDL	OA9-CA7-OA8-CA6
69	1Y	209	3PE	C32-C31-O31-C3
69	1Y	212	3PE	C32-C31-O31-C3
69	1Y	214	3PE	C32-C31-O31-C3
69	1b	101	3PE	C32-C31-O31-C3
69	1d	203	3PE	C32-C31-O31-C3
69	1m	202	3PE	C32-C31-O31-C3
69	1m	203	3PE	C32-C31-O31-C3
69	1o	201	3PE	C32-C31-O31-C3
69	3C	503	3PE	C32-C31-O31-C3
69	3C	511	3PE	C32-C31-O31-C3
69	3G	105	3PE	C32-C31-O31-C3
69	3J	101	3PE	C32-C31-O31-C3
69	3P	504	3PE	C32-C31-O31-C3
69	3P	508	3PE	C32-C31-O31-C3
69	4G	101	3PE	C32-C31-O31-C3
70	1P	502	PC1	C32-C31-O31-C3
75	1L	704	CDL	C71-CB7-OB8-CB6
75	1N	402	CDL	C31-CA7-OA8-CA6
75	1N	402	CDL	C71-CB7-OB8-CB6
75	1d	205	CDL	C31-CA7-OA8-CA6
91	4A	606	PGV	C20-C19-O03-C01
93	4B	303	PSC	C20-C19-O03-C01
69	1Y	209	3PE	O32-C31-O31-C3
69	1k	101	3PE	O32-C31-O31-C3
69	3G	105	3PE	O32-C31-O31-C3
69	3J	101	3PE	O32-C31-O31-C3
70	1h	203	PC1	O32-C31-O31-C3
75	1L	704	CDL	OB9-CB7-OB8-CB6
75	1N	402	CDL	OA9-CA7-OA8-CA6
75	1Y	217	CDL	OB9-CB7-OB8-CB6
69	1Y	209	3PE	O22-C21-O21-C2
69	1m	202	3PE	O22-C21-O21-C2
69	3N	501	3PE	O22-C21-O21-C2
69	3P	503	3PE	O22-C21-O21-C2
70	1d	204	PC1	O22-C21-O21-C2
75	3F	201	CDL	OA7-CA5-OA6-CA4
70	1h	202	PC1	C11-C12-N-C14
75	3T	101	CDL	CA4-CA6-OA8-CA7
75	1L	704	CDL	O1-C1-CB2-OB2

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Mol	Chain	Res	Type	Atoms
75	1g	201	CDL	O1-C1-CA2-OA2
75	3A	501	CDL	O1-C1-CA2-OA2
69	3C	507	3PE	C32-C31-O31-C3
69	3C	514	3PE	C32-C31-O31-C3
69	3C	517	3PE	C32-C31-O31-C3
69	3G	104	3PE	C32-C31-O31-C3
69	3P	506	3PE	C32-C31-O31-C3
69	3P	520	3PE	C32-C31-O31-C3
69	3S	201	3PE	C32-C31-O31-C3
75	3A	501	CDL	C31-CA7-OA8-CA6
75	3X	103	CDL	C71-CB7-OB8-CB6
69	1Y	212	3PE	O32-C31-O31-C3
69	1m	205	3PE	O32-C31-O31-C3
69	3C	511	3PE	O32-C31-O31-C3
69	3R	304	3PE	O32-C31-O31-C3
70	1Y	202	PC1	O32-C31-O31-C3
69	1Y	210	3PE	C22-C21-O21-C2
69	1Y	212	3PE	C22-C21-O21-C2
69	1d	201	3PE	C22-C21-O21-C2
69	1f	104	3PE	C22-C21-O21-C2
69	3C	506	3PE	C22-C21-O21-C2
69	3C	514	3PE	C22-C21-O21-C2
69	3G	107	3PE	C22-C21-O21-C2
69	3G	109	3PE	C22-C21-O21-C2
69	3W	102	3PE	C22-C21-O21-C2
69	3Y	101	3PE	C22-C21-O21-C2
69	3Y	103	3PE	C22-C21-O21-C2
70	1h	202	PC1	C22-C21-O21-C2
70	1h	203	PC1	C22-C21-O21-C2
75	1Y	217	CDL	C11-CA5-OA6-CA4
75	3F	201	CDL	C11-CA5-OA6-CA4
75	4C	307	CDL	C51-CB5-OB6-CB4
69	1m	205	3PE	C32-C31-O31-C3
69	3W	103	3PE	C32-C31-O31-C3
70	1M	501	PC1	C32-C31-O31-C3
70	1Y	202	PC1	C32-C31-O31-C3
70	1h	203	PC1	C32-C31-O31-C3
69	1d	203	3PE	O32-C31-O31-C3
69	1m	202	3PE	O32-C31-O31-C3
69	3P	508	3PE	O32-C31-O31-C3
69	3S	201	3PE	O32-C31-O31-C3
69	4G	101	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
75	3A	501	CDL	OA9-CA7-OA8-CA6
93	4B	303	PSC	O04-C19-O03-C01
70	1h	202	PC1	O22-C21-O21-C2
86	3D	501	HEC	C3D-CAD-CBD-CGD
75	1g	201	CDL	CB4-CB3-OB5-PB2
75	3X	103	CDL	C1-CB2-OB2-PB2
69	1Y	214	3PE	O32-C31-O31-C3
69	1m	203	3PE	O32-C31-O31-C3
69	3G	104	3PE	O32-C31-O31-C3
69	3P	504	3PE	O32-C31-O31-C3
70	1P	502	PC1	O32-C31-O31-C3
75	1N	402	CDL	OB9-CB7-OB8-CB6
69	1f	101	3PE	C32-C31-O31-C3
69	3J	105	3PE	C32-C31-O31-C3
75	1H	401	CDL	C31-CA7-OA8-CA6
75	3N	502	CDL	C31-CA7-OA8-CA6
81	1T	101	EHZ	O3-C12-N1-C11
69	3C	517	3PE	O32-C31-O31-C3
69	3P	506	3PE	O32-C31-O31-C3
69	3P	520	3PE	O32-C31-O31-C3
75	3X	103	CDL	OB9-CB7-OB8-CB6
69	1d	203	3PE	C2D-C2E-C2F-C2G
69	1f	101	3PE	O32-C31-O31-C3
69	3J	105	3PE	O32-C31-O31-C3
75	1H	401	CDL	OA9-CA7-OA8-CA6
75	3N	502	CDL	OA9-CA7-OA8-CA6
75	3X	103	CDL	OA9-CA7-OA8-CA6
69	1Y	212	3PE	O22-C21-O21-C2
69	3G	107	3PE	O22-C21-O21-C2
69	3G	109	3PE	O22-C21-O21-C2
69	3W	102	3PE	O22-C21-O21-C2
69	3Y	101	3PE	O22-C21-O21-C2
70	1h	203	PC1	O22-C21-O21-C2
75	3Y	106	CDL	CB2-C1-CA2-OA2
69	1L	711	3PE	C32-C31-O31-C3
69	1L	712	3PE	C32-C31-O31-C3
69	1N	401	3PE	C32-C31-O31-C3
69	1l	202	3PE	C32-C31-O31-C3
69	3C	509	3PE	C32-C31-O31-C3
69	3C	512	3PE	C32-C31-O31-C3
69	3D	503	3PE	C32-C31-O31-C3
69	3E	302	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	3G	109	3PE	C32-C31-O31-C3
69	3P	507	3PE	C32-C31-O31-C3
69	3P	514	3PE	C32-C31-O31-C3
69	3Q	502	3PE	C32-C31-O31-C3
69	3Q	503	3PE	C32-C31-O31-C3
69	3Q	504	3PE	C32-C31-O31-C3
69	3X	107	3PE	C32-C31-O31-C3
69	3Y	101	3PE	C32-C31-O31-C3
70	1A	202	PC1	C32-C31-O31-C3
75	1g	201	CDL	C31-CA7-OA8-CA6
75	1i	201	CDL	C31-CA7-OA8-CA6
75	1q	202	CDL	C71-CB7-OB8-CB6
75	3D	504	CDL	C71-CB7-OB8-CB6
75	3F	201	CDL	C71-CB7-OB8-CB6
75	3X	103	CDL	C31-CA7-OA8-CA6
75	3Y	106	CDL	C71-CB7-OB8-CB6
91	4A	607	PGV	C20-C19-O03-C01
91	4K	101	PGV	C20-C19-O03-C01
69	1d	201	3PE	C32-C33-C34-C35
69	1l	202	3PE	C33-C34-C35-C36
70	3P	509	PC1	C28-C29-C2A-C2B
70	1Y	206	PC1	C11-C12-N-C13
70	1Y	206	PC1	C11-C12-N-C15
70	1h	202	PC1	C11-C12-N-C13
69	1d	201	3PE	C38-C39-C3A-C3B
69	3A	503	3PE	C35-C36-C37-C38
69	3C	509	3PE	C23-C24-C25-C26
75	1Y	217	CDL	C11-C12-C13-C14
69	1d	201	3PE	C34-C35-C36-C37
79	1P	501	NDP	O4D-C1D-N1N-C6N
75	1L	704	CDL	O1-C1-CA2-OA2
69	1L	710	3PE	C32-C31-O31-C3
91	4C	302	PGV	C20-C19-O03-C01
69	1L	712	3PE	O32-C31-O31-C3
69	3C	512	3PE	O32-C31-O31-C3
75	1i	201	CDL	OA9-CA7-OA8-CA6
69	1o	201	3PE	C31-C32-C33-C34
69	1N	401	3PE	O32-C31-O31-C3
69	1l	202	3PE	O32-C31-O31-C3
69	3C	509	3PE	O32-C31-O31-C3
69	3E	302	3PE	O32-C31-O31-C3
69	3G	109	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	3Q	503	3PE	O32-C31-O31-C3
69	3X	107	3PE	O32-C31-O31-C3
75	1g	201	CDL	OA9-CA7-OA8-CA6
75	1q	202	CDL	OB9-CB7-OB8-CB6
91	4A	607	PGV	O04-C19-O03-C01
69	1Y	210	3PE	O22-C21-O21-C2
69	3C	506	3PE	O22-C21-O21-C2
75	1Y	217	CDL	OA7-CA5-OA6-CA4
69	1L	710	3PE	C22-C21-O21-C2
69	3C	505	3PE	C22-C21-O21-C2
69	1J	201	3PE	O21-C2-C3-O31
69	3J	103	3PE	O21-C2-C3-O31
69	3C	505	3PE	C32-C31-O31-C3
69	1d	201	3PE	C36-C37-C38-C39
69	1L	712	3PE	C2A-C2B-C2C-C2D
77	1O	401	GTP	O4'-C4'-C5'-O5'
69	3G	110	3PE	C32-C31-O31-C3
69	3J	104	3PE	C32-C31-O31-C3
69	3P	517	3PE	C32-C31-O31-C3
70	3T	102	PC1	C23-C24-C25-C26
69	1d	201	3PE	C21-C22-C23-C24
69	3W	103	3PE	C31-C32-C33-C34
70	1J	202	PC1	C21-C22-C23-C24
69	3Y	101	3PE	O32-C31-O31-C3
69	1f	104	3PE	O22-C21-O21-C2
69	3C	514	3PE	O22-C21-O21-C2
88	4A	601	HEA	C19-C20-C21-C22
69	1Y	215	3PE	C36-C37-C38-C39
69	3C	513	3PE	C2-C3-O31-C31
75	1g	201	CDL	CA4-CA6-OA8-CA7
69	1m	201	3PE	C28-C29-C2A-C2B
69	1Y	213	3PE	C31-C32-C33-C34
69	1o	201	3PE	C21-C22-C23-C24
69	3D	502	3PE	C31-C32-C33-C34
69	3P	508	3PE	C21-C22-C23-C24
70	3X	104	PC1	C31-C32-C33-C34
75	1d	205	CDL	CA5-C11-C12-C13
75	1i	201	CDL	CA7-C31-C32-C33
75	3P	513	CDL	CB5-C51-C52-C53
69	3C	505	3PE	O32-C31-O31-C3
69	3P	507	3PE	O32-C31-O31-C3
69	3Q	502	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
70	1A	202	PC1	O32-C31-O31-C3
75	3F	201	CDL	OB9-CB7-OB8-CB6
69	1L	711	3PE	C22-C21-O21-C2
69	3P	519	3PE	C22-C21-O21-C2
91	4A	609	PGV	C2-C1-O01-C02
69	1L	701	3PE	C31-C32-C33-C34
69	1b	101	3PE	C31-C32-C33-C34
69	1e	201	3PE	C21-C22-C23-C24
70	1B	202	PC1	C21-C22-C23-C24
70	3P	509	PC1	C21-C22-C23-C24
75	3D	504	CDL	OB9-CB7-OB8-CB6
91	4K	101	PGV	O04-C19-O03-C01
69	1d	206	3PE	C24-C25-C26-C27
69	1Y	215	3PE	C25-C26-C27-C28
69	1l	204	3PE	C26-C27-C28-C29
75	1i	201	CDL	C13-C14-C15-C16
69	3Y	107	3PE	C36-C37-C38-C39
70	1J	202	PC1	C24-C25-C26-C27
75	1g	201	CDL	O1-C1-CB2-OB2
69	3J	102	3PE	C32-C31-O31-C3
91	4C	303	PGV	C20-C19-O03-C01
69	3C	506	3PE	C27-C28-C29-C2A
69	1L	711	3PE	O32-C31-O31-C3
69	3P	514	3PE	O32-C31-O31-C3
69	3Q	504	3PE	O32-C31-O31-C3
75	3Y	106	CDL	OB9-CB7-OB8-CB6
70	1J	202	PC1	C31-C32-C33-C34
69	3P	519	3PE	O22-C21-O21-C2
69	3Y	103	3PE	O22-C21-O21-C2
75	4C	307	CDL	OB7-CB5-OB6-CB4
69	3G	109	3PE	C22-C23-C24-C25
69	1Y	210	3PE	C23-C24-C25-C26
69	3D	503	3PE	O32-C31-O31-C3
91	4C	302	PGV	O04-C19-O03-C01
75	1L	704	CDL	CA7-C31-C32-C33
69	1d	201	3PE	C27-C28-C29-C2A
75	1q	201	CDL	C17-C18-C19-C20
87	3X	102	PEK	C31-C32-C33-C34
69	1d	206	3PE	C32-C31-O31-C3
69	1g	203	3PE	C32-C31-O31-C3
69	3G	102	3PE	C32-C31-O31-C3
75	1g	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
75	3A	501	CDL	C71-CB7-OB8-CB6
70	1B	202	PC1	C22-C21-O21-C2
69	1L	710	3PE	O32-C31-O31-C3
69	3G	110	3PE	O32-C31-O31-C3
69	1Y	213	3PE	C21-C22-C23-C24
69	1B	204	3PE	C29-C2A-C2B-C2C
69	3P	503	3PE	C39-C3A-C3B-C3C
91	4A	607	PGV	C24-C25-C26-C27
69	1Y	216	3PE	C24-C25-C26-C27
69	1L	711	3PE	O22-C21-O21-C2
69	3C	505	3PE	O22-C21-O21-C2
91	4A	609	PGV	O02-C1-O01-C02
75	1L	704	CDL	CA2-C1-CB2-OB2
75	1g	201	CDL	CA2-C1-CB2-OB2
75	3A	501	CDL	CB2-C1-CA2-OA2
69	1J	201	3PE	C32-C31-O31-C3
69	1L	705	3PE	C32-C31-O31-C3
69	1L	706	3PE	C32-C31-O31-C3
91	4N	101	PGV	C20-C19-O03-C01
69	1m	205	3PE	C32-C33-C34-C35
69	3P	507	3PE	C34-C35-C36-C37
75	1Y	217	CDL	C17-C18-C19-C20
70	1Y	202	PC1	C11-C12-N-C15
70	1d	204	PC1	C11-C12-N-C13
70	1d	204	PC1	C11-C12-N-C14
70	3T	102	PC1	C11-C12-N-C13
70	3T	102	PC1	C11-C12-N-C15
93	4B	303	PSC	C04-C05-N-C06
93	4B	303	PSC	C04-C05-N-C08
69	3G	111	3PE	C31-C32-C33-C34
75	1d	202	CDL	C11-C12-C13-C14
69	1Y	204	3PE	C32-C31-O31-C3
69	1L	710	3PE	C21-C22-C23-C24
70	1H	404	PC1	C3C-C3D-C3E-C3F
69	1L	712	3PE	C22-C21-O21-C2
69	1Y	208	3PE	C22-C21-O21-C2
69	3P	512	3PE	C22-C21-O21-C2
69	3Y	102	3PE	C22-C21-O21-C2
70	1P	502	PC1	C22-C21-O21-C2
70	1Y	206	PC1	C22-C21-O21-C2
70	3X	104	PC1	C22-C21-O21-C2
69	3C	508	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
69	3G	111	3PE	C23-C24-C25-C26
69	1L	712	3PE	O22-C21-O21-C2
69	1Y	208	3PE	O22-C21-O21-C2
69	3X	105	3PE	O22-C21-O21-C2
69	3Y	102	3PE	O22-C21-O21-C2
70	1B	202	PC1	O22-C21-O21-C2
70	1P	502	PC1	O22-C21-O21-C2
70	1Y	206	PC1	O22-C21-O21-C2
70	3X	104	PC1	O22-C21-O21-C2
75	1Y	217	CDL	O1-C1-CA2-OA2
75	4C	306	CDL	C51-C52-C53-C54
69	3X	107	3PE	C21-C22-C23-C24
69	1A	203	3PE	C36-C37-C38-C39
69	3A	502	3PE	C22-C23-C24-C25
69	3P	517	3PE	C27-C28-C29-C2A
69	1Y	204	3PE	C2-C1-O11-P
69	1g	203	3PE	C2-C1-O11-P
69	3G	102	3PE	C2-C1-O11-P
91	4J	101	PGV	C02-C03-O11-P
69	3J	104	3PE	O32-C31-O31-C3
69	1Y	210	3PE	C35-C36-C37-C38
69	1g	202	3PE	C1-C2-O21-C21
69	3J	105	3PE	C1-C2-O21-C21
69	3W	102	3PE	C3-C2-O21-C21
69	3X	105	3PE	C1-C2-O21-C21
69	3X	108	3PE	C1-C2-O21-C21
69	4G	101	3PE	C3-C2-O21-C21
75	1Y	217	CDL	CA3-CA4-OA6-CA5
75	3N	502	CDL	CA3-CA4-OA6-CA5
75	3X	103	CDL	CA3-CA4-OA6-CA5
69	3J	102	3PE	O32-C31-O31-C3
69	3P	517	3PE	O32-C31-O31-C3
69	1h	204	3PE	C35-C36-C37-C38
69	1L	705	3PE	C22-C21-O21-C2
69	3C	510	3PE	C22-C21-O21-C2
69	3X	105	3PE	C22-C21-O21-C2
75	4B	302	CDL	C11-CA5-OA6-CA4
91	4C	302	PGV	C2-C1-O01-C02
88	4A	601	HEA	O11-C11-C12-C13
69	1L	710	3PE	C25-C26-C27-C28
75	1i	201	CDL	C17-C18-C19-C20
75	3N	502	CDL	C59-C60-C61-C62

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Mol	Chain	Res	Type	Atoms
75	3N	502	CDL	C36-C37-C38-C39
69	1Y	216	3PE	C32-C31-O31-C3
69	3G	101	3PE	C32-C31-O31-C3
75	1d	202	CDL	C71-CB7-OB8-CB6
75	1Y	217	CDL	C21-C22-C23-C24
70	1Y	206	PC1	C11-C12-N-C14
70	1d	204	PC1	C11-C12-N-C15
70	3T	102	PC1	C11-C12-N-C14
93	4B	303	PSC	C04-C05-N-C07
69	1m	201	3PE	C35-C36-C37-C38
69	3P	519	3PE	C3E-C3F-C3G-C3H
69	1L	708	3PE	C23-C24-C25-C26
69	1J	201	3PE	O32-C31-O31-C3
75	1g	201	CDL	OB9-CB7-OB8-CB6
69	1Y	213	3PE	C32-C33-C34-C35
69	1d	201	3PE	C24-C25-C26-C27
69	1d	201	3PE	C2C-C2D-C2E-C2F
69	3C	508	3PE	C35-C36-C37-C38
69	3T	103	3PE	C36-C37-C38-C39
70	1M	501	PC1	C28-C29-C2A-C2B
75	1d	205	CDL	C14-C15-C16-C17
69	1L	712	3PE	C33-C34-C35-C36
69	1Y	213	3PE	C39-C3A-C3B-C3C
69	1d	201	3PE	C2A-C2B-C2C-C2D
69	1m	203	3PE	C26-C27-C28-C29
69	3C	508	3PE	C39-C3A-C3B-C3C
70	1B	203	PC1	C29-C2A-C2B-C2C
69	3G	101	3PE	C21-C22-C23-C24
69	1o	201	3PE	C25-C26-C27-C28
69	3R	302	3PE	C22-C23-C24-C25
75	3P	513	CDL	C36-C37-C38-C39
69	1g	203	3PE	O32-C31-O31-C3
69	3G	102	3PE	O32-C31-O31-C3
75	3A	501	CDL	OB9-CB7-OB8-CB6
91	4C	303	PGV	O04-C19-O03-C01
91	4N	101	PGV	O04-C19-O03-C01
69	1B	204	3PE	C32-C31-O31-C3
69	3P	503	3PE	C32-C31-O31-C3
69	1L	708	3PE	C28-C29-C2A-C2B
69	1Y	213	3PE	C3C-C3D-C3E-C3F
69	3G	105	3PE	C25-C26-C27-C28
69	3R	302	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
69	3S	201	3PE	C35-C36-C37-C38
75	1d	202	CDL	C31-C32-C33-C34
75	4B	302	CDL	C62-C63-C64-C65
91	4C	304	PGV	C5-C6-C7-C8
69	3P	512	3PE	O22-C21-O21-C2
75	4B	302	CDL	OA7-CA5-OA6-CA4
69	1d	203	3PE	C33-C34-C35-C36
70	1B	203	PC1	C24-C25-C26-C27
70	1J	202	PC1	C35-C36-C37-C38
87	3X	102	PEK	C25-C26-C27-C28
75	3X	103	CDL	C14-C15-C16-C17
75	3P	513	CDL	CA4-CA6-OA8-CA7
69	1d	206	3PE	O32-C31-O31-C3
69	1Y	205	3PE	C2A-C2B-C2C-C2D
69	3G	111	3PE	C24-C25-C26-C27
69	3X	106	3PE	C2B-C2C-C2D-C2E
69	1L	703	3PE	C22-C21-O21-C2
70	3P	509	PC1	C22-C21-O21-C2
70	3R	303	PC1	C22-C21-O21-C2
69	1N	401	3PE	C22-C23-C24-C25
69	1d	203	3PE	C2C-C2D-C2E-C2F
69	1Y	211	3PE	C2A-C2B-C2C-C2D
69	1Y	213	3PE	C2B-C2C-C2D-C2E
69	1l	202	3PE	C35-C36-C37-C38
75	1g	201	CDL	C57-C58-C59-C60
69	3W	102	3PE	C31-C32-C33-C34
77	1O	401	GTP	C3'-C4'-C5'-O5'
69	3P	506	3PE	C34-C35-C36-C37
75	3A	501	CDL	C61-C62-C63-C64
69	1L	706	3PE	O32-C31-O31-C3
69	1L	702	3PE	C2-C3-O31-C31
69	1L	705	3PE	O32-C31-O31-C3
69	1Y	204	3PE	O32-C31-O31-C3
69	1d	203	3PE	C23-C24-C25-C26
69	1k	101	3PE	C32-C33-C34-C35
69	1o	201	3PE	C3C-C3D-C3E-C3F
75	1g	201	CDL	C36-C37-C38-C39
91	4C	302	PGV	O02-C1-O01-C02
75	1g	201	CDL	C37-C38-C39-C40
91	4J	101	PGV	C20-C21-C22-C23
75	1Y	217	CDL	CB2-C1-CA2-OA2
69	3X	108	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
75	1q	202	CDL	C31-CA7-OA8-CA6
75	3Y	106	CDL	C31-CA7-OA8-CA6
75	4C	306	CDL	C31-CA7-OA8-CA6
69	1f	101	3PE	C1-C2-C3-O31
69	1Y	209	3PE	C32-C33-C34-C35
69	3G	101	3PE	C3A-C3B-C3C-C3D
70	1d	204	PC1	C31-C32-C33-C34
93	4B	303	PSC	C1-C2-C3-C4
69	1L	702	3PE	C22-C23-C24-C25
69	1Y	201	3PE	C36-C37-C38-C39
69	1Y	213	3PE	C22-C23-C24-C25
69	1d	201	3PE	C33-C34-C35-C36
69	1d	201	3PE	C28-C29-C2A-C2B
69	1e	201	3PE	C22-C23-C24-C25
69	1m	202	3PE	C23-C24-C25-C26
69	3X	106	3PE	C27-C28-C29-C2A
69	4G	104	3PE	C22-C23-C24-C25
70	3J	106	PC1	C23-C24-C25-C26
75	4C	306	CDL	C75-C76-C77-C78
69	1m	202	3PE	C22-C23-C24-C25
69	3G	109	3PE	C33-C34-C35-C36
69	3X	107	3PE	C34-C35-C36-C37
70	3R	303	PC1	C36-C37-C38-C39
75	1N	402	CDL	C34-C35-C36-C37
75	1Y	217	CDL	C39-C40-C41-C42
70	1Y	202	PC1	C11-C12-N-C14
70	1h	202	PC1	C11-C12-N-C15
70	3J	106	PC1	C11-C12-N-C15
70	3X	104	PC1	C11-C12-N-C14
70	1B	202	PC1	C22-C23-C24-C25
70	3X	104	PC1	C35-C36-C37-C38
75	4C	306	CDL	C17-C18-C19-C20
69	3C	507	3PE	C3A-C3B-C3C-C3D
69	3S	201	3PE	C2E-C2F-C2G-C2H
70	1H	403	PC1	C28-C29-C2A-C2B
75	1Y	217	CDL	C81-C82-C83-C84
75	1g	201	CDL	C63-C64-C65-C66
69	1Y	214	3PE	C22-C21-O21-C2
70	1H	402	PC1	C22-C21-O21-C2
69	1d	201	3PE	C29-C2A-C2B-C2C
70	3X	104	PC1	C26-C27-C28-C29
69	1B	204	3PE	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
69	1Y	216	3PE	O32-C31-O31-C3
69	3G	101	3PE	O32-C31-O31-C3
69	3P	503	3PE	O32-C31-O31-C3
75	1q	202	CDL	OA9-CA7-OA8-CA6
69	1N	401	3PE	C23-C24-C25-C26
69	3W	101	3PE	C23-C24-C25-C26
69	1L	703	3PE	O22-C21-O21-C2
69	3C	510	3PE	O22-C21-O21-C2
70	3P	509	PC1	O22-C21-O21-C2
70	3R	303	PC1	O22-C21-O21-C2
87	3X	102	PEK	O02-C1-O01-C02
69	1o	201	3PE	C2B-C2C-C2D-C2E
70	3X	104	PC1	C2B-C2C-C2D-C2E
69	3G	101	3PE	C25-C26-C27-C28
69	3W	102	3PE	C3A-C3B-C3C-C3D
69	3X	105	3PE	C36-C37-C38-C39
70	1B	202	PC1	C24-C25-C26-C27
75	3X	103	CDL	C75-C76-C77-C78
75	4B	302	CDL	C59-C60-C61-C62
69	1f	103	3PE	C32-C31-O31-C3
69	3N	503	3PE	C32-C31-O31-C3
87	3X	102	PEK	C22-C21-O03-C01
69	1Y	208	3PE	C34-C35-C36-C37
69	1Y	213	3PE	C2A-C2B-C2C-C2D
69	3P	508	3PE	C29-C2A-C2B-C2C
70	1h	203	PC1	C34-C35-C36-C37
70	3R	303	PC1	C2A-C2B-C2C-C2D
75	1g	201	CDL	C53-C54-C55-C56
75	3N	502	CDL	C17-C18-C19-C20
75	3Y	106	CDL	C73-C74-C75-C76
87	3X	102	PEK	C23-C24-C25-C26
69	1L	709	3PE	C22-C23-C24-C25
69	1d	203	3PE	C36-C37-C38-C39
69	3P	514	3PE	C37-C38-C39-C3A
69	3P	520	3PE	C22-C23-C24-C25
69	3Y	102	3PE	C23-C24-C25-C26
75	1Y	217	CDL	C74-C75-C76-C77
69	1k	101	3PE	C29-C2A-C2B-C2C
69	1d	206	3PE	C22-C23-C24-C25
69	3X	108	3PE	C32-C33-C34-C35
70	1d	204	PC1	C37-C38-C39-C3A
70	3T	102	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
69	3X	101	3PE	C2A-C2B-C2C-C2D
91	4A	609	PGV	C20-C19-O03-C01
87	3X	102	PEK	C35-C36-C37-C38
69	1A	201	3PE	C22-C21-O21-C2
69	1A	203	3PE	C22-C21-O21-C2
69	1B	204	3PE	C22-C21-O21-C2
69	1f	101	3PE	C22-C21-O21-C2
69	3C	504	3PE	C22-C21-O21-C2
69	3G	102	3PE	C22-C21-O21-C2
69	3P	507	3PE	C22-C21-O21-C2
69	3R	302	3PE	C22-C21-O21-C2
69	3X	108	3PE	C22-C21-O21-C2
69	3Y	104	3PE	C22-C21-O21-C2
70	1B	203	PC1	C22-C21-O21-C2
70	1J	202	PC1	C22-C21-O21-C2
75	1N	402	CDL	C51-CB5-OB6-CB4
75	1d	202	CDL	C11-CA5-OA6-CA4
75	3P	513	CDL	C51-CB5-OB6-CB4
87	3X	102	PEK	C2-C1-O01-C02
91	4A	607	PGV	C2-C1-O01-C02
91	4N	101	PGV	C2-C1-O01-C02
69	1Y	211	3PE	C21-C22-C23-C24
69	1m	201	3PE	C21-C22-C23-C24
87	4G	103	PEK	C21-C22-C23-C24
69	1d	206	3PE	C37-C38-C39-C3A
69	1L	705	3PE	O22-C21-O21-C2
70	1B	203	PC1	O22-C21-O21-C2
75	1Y	217	CDL	C83-C84-C85-C86
75	1d	205	CDL	C23-C24-C25-C26
69	1L	702	3PE	C25-C26-C27-C28
70	1H	402	PC1	C32-C33-C34-C35
69	1A	201	3PE	C32-C33-C34-C35
69	3J	103	3PE	C21-C22-C23-C24
69	1L	710	3PE	C23-C24-C25-C26
69	3C	512	3PE	C25-C26-C27-C28
75	4B	302	CDL	C51-C52-C53-C54
75	4B	302	CDL	C58-C59-C60-C61
75	1N	402	CDL	C31-C32-C33-C34
85	3C	502	HEM	C2C-C3C-CAC-CBC
85	3P	501	HEM	C2B-C3B-CAB-CBB
70	1Y	202	PC1	C11-C12-N-C13
70	3P	509	PC1	C11-C12-N-C15

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Mol	Chain	Res	Type	Atoms
69	1B	205	3PE	C31-C32-C33-C34
69	3P	508	3PE	C34-C35-C36-C37
69	3T	103	3PE	C28-C29-C2A-C2B
69	1J	201	3PE	C3A-C3B-C3C-C3D
69	3G	104	3PE	C23-C24-C25-C26
69	3Q	503	3PE	C22-C23-C24-C25
69	1d	203	3PE	C27-C28-C29-C2A
69	1f	104	3PE	C24-C25-C26-C27
69	3C	509	3PE	C28-C29-C2A-C2B
69	3Y	101	3PE	C3A-C3B-C3C-C3D
75	4C	306	CDL	C61-C62-C63-C64
69	3X	108	3PE	O32-C31-O31-C3
75	1d	202	CDL	OB9-CB7-OB8-CB6
75	4C	306	CDL	OA9-CA7-OA8-CA6
69	1N	401	3PE	C36-C37-C38-C39
69	3A	502	3PE	C32-C33-C34-C35
75	1q	202	CDL	CA5-C11-C12-C13
69	1Y	214	3PE	O22-C21-O21-C2
69	1f	101	3PE	O22-C21-O21-C2
69	3Y	104	3PE	O22-C21-O21-C2
70	1J	202	PC1	O22-C21-O21-C2
69	3C	509	3PE	O11-C1-C2-O21
69	3C	510	3PE	O11-C1-C2-O21
69	3R	302	3PE	O11-C1-C2-O21
91	4G	102	PGV	O01-C02-C03-O11
70	3X	104	PC1	C2D-C2E-C2F-C2G
69	1L	701	3PE	C22-C21-O21-C2
69	1m	204	3PE	C22-C21-O21-C2
70	1H	403	PC1	C22-C21-O21-C2
85	3C	501	HEM	C4B-C3B-CAB-CBB
85	3C	502	HEM	C4B-C3B-CAB-CBB
85	3P	502	HEM	C4B-C3B-CAB-CBB
69	1Y	215	3PE	C22-C23-C24-C25
69	1l	202	3PE	C32-C33-C34-C35
69	3C	504	3PE	C34-C35-C36-C37
69	3J	104	3PE	C2C-C2D-C2E-C2F
91	4A	609	PGV	C21-C22-C23-C24
69	1L	702	3PE	C21-C22-C23-C24
69	3C	504	3PE	C21-C22-C23-C24
69	3C	514	3PE	C21-C22-C23-C24
69	3P	507	3PE	C31-C32-C33-C34
70	1A	202	PC1	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
91	4A	606	PGV	C19-C20-C21-C22
75	3N	502	CDL	OA6-CA4-CA6-OA8
69	1d	201	3PE	C25-C26-C27-C28
69	3E	302	3PE	C2A-C2B-C2C-C2D
75	4B	302	CDL	C14-C15-C16-C17
91	4C	303	PGV	C11-C12-C13-C14
70	1h	203	PC1	C32-C33-C34-C35
75	4B	302	CDL	C74-C75-C76-C77
75	3Y	106	CDL	CB4-CB3-OB5-PB2
69	1f	104	3PE	C36-C37-C38-C39
69	3C	505	3PE	C3C-C3D-C3E-C3F
91	4A	609	PGV	C4-C5-C6-C7
91	4K	101	PGV	C3-C4-C5-C6
69	1A	201	3PE	O22-C21-O21-C2
69	1B	204	3PE	O22-C21-O21-C2
69	3G	102	3PE	O22-C21-O21-C2
69	3X	108	3PE	O22-C21-O21-C2
91	4N	101	PGV	O02-C1-O01-C02
75	1g	201	CDL	CB2-C1-CA2-OA2
69	1Y	214	3PE	C28-C29-C2A-C2B
69	1l	203	3PE	C23-C24-C25-C26
70	1J	202	PC1	C34-C35-C36-C37
75	1L	704	CDL	C13-C14-C15-C16
91	4G	102	PGV	C2-C3-C4-C5
69	3P	505	3PE	C32-C31-O31-C3
69	1m	204	3PE	C33-C34-C35-C36
69	1m	204	3PE	C27-C28-C29-C2A
75	4C	306	CDL	C12-C13-C14-C15
69	1l	204	3PE	C2-C3-O31-C31
69	3P	514	3PE	C2-C3-O31-C31
75	3T	101	CDL	C54-C55-C56-C57
69	3C	507	3PE	C21-C22-C23-C24
70	1J	202	PC1	C36-C37-C38-C39
69	1k	101	3PE	C35-C36-C37-C38
69	1f	103	3PE	O32-C31-O31-C3
69	3N	503	3PE	O32-C31-O31-C3
75	3Y	106	CDL	OA9-CA7-OA8-CA6
69	1Y	214	3PE	C35-C36-C37-C38
69	1L	702	3PE	C32-C33-C34-C35
75	3F	201	CDL	C71-C72-C73-C74
81	1T	101	EHZ	O4-C15-C16-O5
69	1L	712	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
69	1g	202	3PE	C27-C28-C29-C2A
69	3G	111	3PE	C32-C33-C34-C35
69	1Y	213	3PE	C26-C27-C28-C29
69	1h	204	3PE	C37-C38-C39-C3A
69	1h	204	3PE	C3B-C3C-C3D-C3E
70	3T	102	PC1	C33-C34-C35-C36
69	1L	711	3PE	O11-C1-C2-C3
69	1M	502	3PE	O11-C1-C2-C3
69	3G	108	3PE	O11-C1-C2-C3
69	3P	510	3PE	O11-C1-C2-C3
75	1L	704	CDL	OA5-CA3-CA4-CA6
91	4G	102	PGV	C01-C02-C03-O11
69	1A	203	3PE	O22-C21-O21-C2
69	3C	504	3PE	O22-C21-O21-C2
69	3P	507	3PE	O22-C21-O21-C2
70	1H	402	PC1	O22-C21-O21-C2
91	4A	607	PGV	O02-C1-O01-C02
69	1L	706	3PE	C22-C23-C24-C25
70	1Y	206	PC1	C27-C28-C29-C2A
75	4C	306	CDL	C38-C39-C40-C41
69	1Y	211	3PE	C32-C33-C34-C35
69	3C	503	3PE	C2C-C2D-C2E-C2F
91	4A	609	PGV	O04-C19-O03-C01
69	1N	401	3PE	C2B-C2C-C2D-C2E
75	1d	205	CDL	C51-CB5-OB6-CB4
75	1q	202	CDL	C51-CB5-OB6-CB4
70	3R	303	PC1	C25-C26-C27-C28
69	3E	302	3PE	C31-C32-C33-C34
69	3C	516	3PE	C38-C39-C3A-C3B
69	3E	303	3PE	C26-C27-C28-C29
69	3W	103	3PE	C2C-C2D-C2E-C2F
69	1A	203	3PE	C32-C31-O31-C3
69	1L	702	3PE	C32-C31-O31-C3
69	1L	701	3PE	C38-C39-C3A-C3B
69	3S	201	3PE	C34-C35-C36-C37
69	3Y	101	3PE	C37-C38-C39-C3A
69	1N	401	3PE	C2A-C2B-C2C-C2D
69	3C	509	3PE	C38-C39-C3A-C3B
75	1q	202	CDL	C73-C74-C75-C76
75	1N	402	CDL	OB7-CB5-OB6-CB4
69	3Y	107	3PE	C23-C24-C25-C26
70	1Y	206	PC1	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
69	3C	513	3PE	C31-C32-C33-C34
69	1J	201	3PE	C1-C2-C3-O31
69	1L	705	3PE	C1-C2-C3-O31
69	1Y	214	3PE	C1-C2-C3-O31
69	1d	203	3PE	C1-C2-C3-O31
69	3G	111	3PE	C1-C2-C3-O31
69	3J	103	3PE	C1-C2-C3-O31
70	1H	404	PC1	C1-C2-C3-O31
75	1d	205	CDL	CB3-CB4-CB6-OB8
75	3N	502	CDL	CA3-CA4-CA6-OA8
75	3Y	106	CDL	CB3-CB4-CB6-OB8
69	1g	202	3PE	C22-C23-C24-C25
69	1l	204	3PE	C32-C33-C34-C35
75	4B	302	CDL	C31-C32-C33-C34
69	1Y	213	3PE	C33-C34-C35-C36
69	3P	506	3PE	C32-C33-C34-C35
70	3J	106	PC1	C27-C28-C29-C2A
69	3S	201	3PE	C32-C33-C34-C35
75	1d	205	CDL	C11-C12-C13-C14
69	3C	504	3PE	C32-C31-O31-C3
69	3P	516	3PE	C32-C31-O31-C3
69	3J	101	3PE	C21-C22-C23-C24
75	1d	205	CDL	CB5-C51-C52-C53
69	1Y	209	3PE	C28-C29-C2A-C2B
69	1Y	214	3PE	C34-C35-C36-C37
69	3J	102	3PE	C22-C23-C24-C25
87	3X	102	PEK	O04-C21-O03-C01
69	3Y	101	3PE	C38-C39-C3A-C3B
75	1q	202	CDL	C33-C34-C35-C36
70	3X	104	PC1	C11-C12-N-C15
69	3P	516	3PE	C31-C32-C33-C34
75	1q	201	CDL	CB5-C51-C52-C53
69	1L	703	3PE	C24-C25-C26-C27
75	4C	307	CDL	C20-C21-C22-C23
69	3C	509	3PE	C2-C1-O11-P
69	3P	504	3PE	C2-C1-O11-P
91	4A	607	PGV	C05-C04-O12-P
69	1L	701	3PE	O22-C21-O21-C2
69	1f	101	3PE	C39-C3A-C3B-C3C
69	3J	101	3PE	C24-C25-C26-C27
88	4A	602	HEA	C2A-CAA-CBA-CGA
69	1d	201	3PE	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
69	1k	101	3PE	C23-C24-C25-C26
69	3Q	504	3PE	C26-C27-C28-C29
75	1d	205	CDL	C71-C72-C73-C74
75	3A	501	CDL	C31-C32-C33-C34
69	3N	503	3PE	C28-C29-C2A-C2B
69	3P	512	3PE	C34-C35-C36-C37
75	1L	704	CDL	C12-C13-C14-C15
69	3P	505	3PE	C31-C32-C33-C34
69	3E	303	3PE	C38-C39-C3A-C3B
69	1A	201	3PE	C32-C31-O31-C3
70	1H	402	PC1	C32-C31-O31-C3
75	1q	201	CDL	C71-CB7-OB8-CB6
69	1Y	216	3PE	C1-C2-O21-C21
69	3G	107	3PE	C3-C2-O21-C21
69	3J	101	3PE	C1-C2-O21-C21
69	3S	201	3PE	C1-C2-O21-C21
69	3X	106	3PE	C3-C2-O21-C21
70	1M	501	PC1	C3-C2-O21-C21
87	3X	102	PEK	C03-C02-O01-C1
75	1N	402	CDL	C55-C56-C57-C58
69	1Y	201	3PE	C39-C3A-C3B-C3C
69	1d	201	3PE	C37-C38-C39-C3A
69	3G	111	3PE	C38-C39-C3A-C3B
69	1Y	213	3PE	C2F-C2G-C2H-C2I
69	1Y	213	3PE	C37-C38-C39-C3A
69	1g	202	3PE	C25-C26-C27-C28
69	3W	101	3PE	C27-C28-C29-C2A
69	1l	203	3PE	C22-C23-C24-C25
69	3X	101	3PE	C32-C33-C34-C35
70	1B	202	PC1	C27-C28-C29-C2A
69	1Y	210	3PE	O11-C1-C2-O21
69	3G	109	3PE	O11-C1-C2-O21
75	1g	201	CDL	OA5-CA3-CA4-OA6
69	1Z	201	3PE	C38-C39-C3A-C3B
69	1f	102	3PE	C32-C31-O31-C3
69	1f	104	3PE	C32-C31-O31-C3
69	3P	512	3PE	C32-C31-O31-C3
69	3P	515	3PE	C32-C31-O31-C3
70	1Y	206	PC1	C32-C31-O31-C3
69	1A	203	3PE	O32-C31-O31-C3
69	3P	505	3PE	O32-C31-O31-C3
69	1d	201	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
69	1e	201	3PE	C29-C2A-C2B-C2C
69	3D	503	3PE	C3C-C3D-C3E-C3F
69	1Y	215	3PE	C34-C35-C36-C37
75	1Y	217	CDL	C35-C36-C37-C38
69	3R	304	3PE	C39-C3A-C3B-C3C
69	1A	201	3PE	C33-C34-C35-C36
69	3Q	503	3PE	C23-C24-C25-C26
70	1H	402	PC1	C3C-C3D-C3E-C3F
75	3F	201	CDL	C35-C36-C37-C38
69	1Y	210	3PE	O21-C2-C3-O31
69	3Q	502	3PE	O21-C2-C3-O31
69	3W	103	3PE	O21-C2-C3-O31
75	1N	402	CDL	OA6-CA4-CA6-OA8
75	3N	502	CDL	C39-C40-C41-C42
69	1J	201	3PE	C35-C36-C37-C38
69	1Y	213	3PE	C35-C36-C37-C38
69	1d	203	3PE	C37-C38-C39-C3A
69	1f	102	3PE	C25-C26-C27-C28
70	1J	202	PC1	C22-C23-C24-C25
70	3P	509	PC1	C11-C12-N-C14
69	1A	203	3PE	C2A-C2B-C2C-C2D
69	3P	506	3PE	C38-C39-C3A-C3B
69	3C	515	3PE	C36-C37-C38-C39
70	1B	202	PC1	C25-C26-C27-C28
69	3X	101	3PE	C3F-C3G-C3H-C3I
75	1d	202	CDL	OA7-CA5-OA6-CA4
69	3C	505	3PE	C28-C29-C2A-C2B
69	3S	201	3PE	C31-C32-C33-C34
69	1m	204	3PE	C3A-C3B-C3C-C3D
87	4G	103	PEK	C22-C23-C24-C25
70	3P	509	PC1	C32-C31-O31-C3
69	3P	508	3PE	C2F-C2G-C2H-C2I
69	3G	101	3PE	C22-C21-O21-C2
75	3D	504	CDL	C51-CB5-OB6-CB4
70	1Y	207	PC1	C24-C25-C26-C27
75	3F	201	CDL	CB5-C51-C52-C53
75	1Y	217	CDL	C79-C80-C81-C82
69	1L	706	3PE	C23-C24-C25-C26
69	3C	508	3PE	C3C-C3D-C3E-C3F
69	3G	111	3PE	C32-C31-O31-C3
69	3P	518	3PE	C32-C31-O31-C3
69	3Y	105	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
91	4J	101	PGV	C20-C19-O03-C01
69	1Y	209	3PE	C38-C39-C3A-C3B
69	3C	509	3PE	C25-C26-C27-C28
69	3C	515	3PE	C34-C35-C36-C37
70	1h	203	PC1	C3B-C3C-C3D-C3E
69	1d	203	3PE	C2B-C2C-C2D-C2E
69	3P	510	3PE	C2D-C2E-C2F-C2G
69	1d	206	3PE	C2D-C2E-C2F-C2G
69	1f	102	3PE	C35-C36-C37-C38
70	1Y	206	PC1	C26-C27-C28-C29
69	1M	502	3PE	C2-C1-O11-P
69	1Y	214	3PE	C2-C1-O11-P
69	1Y	215	3PE	C2-C1-O11-P
75	1g	201	CDL	C1-CB2-OB2-PB2
75	3Y	106	CDL	C1-CA2-OA2-PA1
75	3Y	106	CDL	CA4-CA3-OA5-PA1
75	4C	306	CDL	CB4-CB3-OB5-PB2
91	4C	304	PGV	C02-C03-O11-P
69	1d	206	3PE	C2C-C2D-C2E-C2F
69	3Q	503	3PE	C36-C37-C38-C39
69	1d	203	3PE	C3B-C3C-C3D-C3E
69	3J	104	3PE	C21-C22-C23-C24
69	3P	518	3PE	C27-C28-C29-C2A
69	3Y	104	3PE	C23-C24-C25-C26
91	4K	101	PGV	C27-C28-C29-C30
69	3C	512	3PE	C36-C37-C38-C39
70	3J	106	PC1	C2A-C2B-C2C-C2D
70	1B	202	PC1	C28-C29-C2A-C2B
69	1Y	216	3PE	O11-C1-C2-C3
69	1g	203	3PE	O11-C1-C2-C3
69	1o	201	3PE	O11-C1-C2-C3
69	3C	509	3PE	O11-C1-C2-C3
69	3C	510	3PE	O11-C1-C2-C3
69	3D	502	3PE	O11-C1-C2-C3
69	3G	109	3PE	O11-C1-C2-C3
69	3R	302	3PE	O11-C1-C2-C3
75	1g	201	CDL	OB5-CB3-CB4-CB6
75	3X	103	CDL	OB5-CB3-CB4-CB6
75	3Y	106	CDL	OB5-CB3-CB4-CB6
69	3P	519	3PE	C36-C37-C38-C39
69	3R	302	3PE	C27-C28-C29-C2A
69	3G	102	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
69	1L	701	3PE	C21-C22-C23-C24
69	1Y	210	3PE	C31-C32-C33-C34
69	3G	104	3PE	C21-C22-C23-C24
75	1q	202	CDL	CB7-C71-C72-C73
82	1Y	203	PGT	C45-C46-C47-C48
75	3T	101	CDL	C74-C75-C76-C77
69	3R	302	3PE	O22-C21-O21-C2
81	1n	201	EHZ	N2-C15-C16-C17
69	1o	201	3PE	C33-C34-C35-C36
75	3X	103	CDL	C73-C74-C75-C76
75	3Y	106	CDL	C15-C16-C17-C18
69	1L	702	3PE	O32-C31-O31-C3
69	3P	516	3PE	O32-C31-O31-C3
69	1Y	205	3PE	C26-C27-C28-C29
69	1B	204	3PE	C34-C35-C36-C37
69	1m	203	3PE	C24-C25-C26-C27
87	3X	102	PEK	C24-C25-C26-C27
69	3Q	504	3PE	C34-C35-C36-C37
69	1Y	213	3PE	C29-C2A-C2B-C2C
70	3R	303	PC1	C24-C25-C26-C27
75	4C	307	CDL	C18-C19-C20-C21
69	1d	203	3PE	C3A-C3B-C3C-C3D
75	1N	402	CDL	C33-C34-C35-C36
69	1A	201	3PE	O32-C31-O31-C3
70	3X	104	PC1	C27-C28-C29-C2A
75	1d	202	CDL	C40-C41-C42-C43
69	1l	203	3PE	C26-C27-C28-C29
69	1Y	213	3PE	C3B-C3C-C3D-C3E
69	3P	510	3PE	C27-C28-C29-C2A
69	3P	515	3PE	C26-C27-C28-C29
75	1q	201	CDL	C51-C52-C53-C54
69	1J	201	3PE	C39-C3A-C3B-C3C
69	3C	512	3PE	C2D-C2E-C2F-C2G
70	3X	104	PC1	C3B-C3C-C3D-C3E
75	1d	205	CDL	C82-C83-C84-C85
93	4B	303	PSC	C23-C24-C25-C26
69	1L	711	3PE	C23-C24-C25-C26
69	1b	101	3PE	C32-C33-C34-C35
69	1L	708	3PE	C1-C2-C3-O31
69	3C	510	3PE	C1-C2-C3-O31
69	3Y	104	3PE	C1-C2-C3-O31
75	1L	704	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
75	1N	402	CDL	CB3-CB4-CB6-OB8
75	3D	504	CDL	CB3-CB4-CB6-OB8
75	3T	101	CDL	CB3-CB4-CB6-OB8
75	3T	101	CDL	C31-C32-C33-C34
69	1Y	208	3PE	C35-C36-C37-C38
69	1d	201	3PE	C35-C36-C37-C38
75	3A	501	CDL	C59-C60-C61-C62
69	3C	504	3PE	O32-C31-O31-C3
69	1L	711	3PE	C2B-C2C-C2D-C2E
69	1N	401	3PE	C3B-C3C-C3D-C3E
69	1Y	201	3PE	C33-C34-C35-C36
69	3P	517	3PE	C22-C23-C24-C25
70	3T	102	PC1	C24-C25-C26-C27
75	1q	202	CDL	C39-C40-C41-C42
75	3P	513	CDL	C35-C36-C37-C38
82	1Y	203	PGT	C13-C14-C15-C16
69	3N	503	3PE	C26-C27-C28-C29
69	3C	505	3PE	C2B-C2C-C2D-C2E
69	3P	518	3PE	O32-C31-O31-C3
75	1q	201	CDL	OB9-CB7-OB8-CB6
69	3C	511	3PE	C22-C23-C24-C25
69	1N	401	3PE	C3A-C3B-C3C-C3D
69	1Y	213	3PE	C38-C39-C3A-C3B
75	1Y	217	CDL	C42-C43-C44-C45
70	1H	403	PC1	O22-C21-O21-C2
75	1d	205	CDL	OB7-CB5-OB6-CB4
69	1L	705	3PE	C31-C32-C33-C34
69	1Y	216	3PE	O11-C1-C2-O21
69	1o	201	3PE	O11-C1-C2-O21
69	3D	502	3PE	O11-C1-C2-O21
70	1M	501	PC1	O11-C1-C2-O21
75	1Y	217	CDL	OB5-CB3-CB4-OB6
69	3Y	105	3PE	C22-C21-O21-C2
69	1f	104	3PE	C2-C1-O11-P
69	1m	201	3PE	C2-C1-O11-P
69	3J	103	3PE	C2-C1-O11-P
69	3P	515	3PE	C2-C1-O11-P
69	3W	101	3PE	C2-C1-O11-P
69	3W	103	3PE	C2-C1-O11-P
75	1q	202	CDL	C1-CA2-OA2-PA1
75	3P	513	CDL	C1-CB2-OB2-PB2
75	3X	103	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
69	1d	203	3PE	C35-C36-C37-C38
69	1f	104	3PE	C26-C27-C28-C29
83	1h	201	AME	C-CA-N-CT1
69	1g	202	3PE	C2A-C2B-C2C-C2D
69	3G	106	3PE	C24-C25-C26-C27
69	1m	203	3PE	C35-C36-C37-C38
69	3C	503	3PE	C36-C37-C38-C39
69	3P	508	3PE	C3B-C3C-C3D-C3E
70	1Y	206	PC1	C36-C37-C38-C39
70	3P	509	PC1	C35-C36-C37-C38
75	1q	202	CDL	C17-C18-C19-C20
69	3P	520	3PE	C21-C22-C23-C24
69	1Y	214	3PE	O21-C2-C3-O31
69	1g	202	3PE	O21-C2-C3-O31
69	1l	202	3PE	O21-C2-C3-O31
69	3P	506	3PE	O21-C2-C3-O31
69	3R	302	3PE	O21-C2-C3-O31
69	3X	101	3PE	O21-C2-C3-O31
69	3X	108	3PE	O21-C2-C3-O31
75	1H	401	CDL	OA6-CA4-CA6-OA8
75	1N	402	CDL	OB6-CB4-CB6-OB8
75	1g	201	CDL	OA6-CA4-CA6-OA8
75	3D	504	CDL	OB6-CB4-CB6-OB8
87	4G	103	PEK	C9-C10-C11-C12
87	4G	103	PEK	C12-C13-C14-C15
93	4B	303	PSC	C9-C10-C11-C12
69	1m	201	3PE	C3B-C3C-C3D-C3E
69	3A	503	3PE	C29-C2A-C2B-C2C
69	3C	507	3PE	C2C-C2D-C2E-C2F
69	3Y	102	3PE	C33-C34-C35-C36
75	3N	502	CDL	C80-C81-C82-C83
69	1A	203	3PE	C21-C22-C23-C24
69	3J	102	3PE	C21-C22-C23-C24
75	4C	306	CDL	CA5-C11-C12-C13
69	1M	502	3PE	C22-C23-C24-C25
69	3R	305	3PE	C22-C23-C24-C25
69	1L	711	3PE	C26-C27-C28-C29
69	3P	515	3PE	C2C-C2D-C2E-C2F
69	3J	101	3PE	C35-C36-C37-C38
69	3P	520	3PE	C34-C35-C36-C37
69	3R	305	3PE	C3B-C3C-C3D-C3E
69	3W	102	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
69	1L	702	3PE	C31-C32-C33-C34
69	1d	201	3PE	C31-C32-C33-C34
69	1B	205	3PE	C37-C38-C39-C3A
70	1M	501	PC1	C29-C2A-C2B-C2C
75	1d	205	CDL	C60-C61-C62-C63
69	1f	102	3PE	O32-C31-O31-C3
69	1Y	213	3PE	C3E-C3F-C3G-C3H
70	3P	509	PC1	C38-C39-C3A-C3B
69	3E	303	3PE	C39-C3A-C3B-C3C
69	1f	104	3PE	O32-C31-O31-C3
69	3P	512	3PE	O32-C31-O31-C3
69	3C	505	3PE	C39-C3A-C3B-C3C
75	3X	103	CDL	C77-C78-C79-C80
69	1L	702	3PE	C23-C24-C25-C26
69	3D	503	3PE	C24-C25-C26-C27
70	1h	203	PC1	C24-C25-C26-C27
69	1L	708	3PE	C22-C23-C24-C25
75	3P	513	CDL	OB7-CB5-OB6-CB4
69	1Y	210	3PE	C32-C33-C34-C35
69	1Y	216	3PE	C26-C27-C28-C29
69	1g	202	3PE	C37-C38-C39-C3A
69	3J	101	3PE	C28-C29-C2A-C2B
75	3X	103	CDL	O1-C1-CB2-OB2
69	3R	302	3PE	C3A-C3B-C3C-C3D
75	3A	501	CDL	C83-C84-C85-C86
69	1f	101	3PE	C35-C36-C37-C38
69	1g	203	3PE	C22-C21-O21-C2
82	1Y	203	PGT	C31-C32-C33-C34
82	1Y	203	PGT	C18-C19-C20-C21
69	3R	304	3PE	C27-C28-C29-C2A
75	1d	202	CDL	C14-C15-C16-C17
69	1M	502	3PE	C2D-C2E-C2F-C2G
69	3E	302	3PE	C24-C25-C26-C27
75	3A	501	CDL	C22-C23-C24-C25
69	3P	507	3PE	C21-C22-C23-C24
69	1N	401	3PE	C29-C2A-C2B-C2C
69	1e	201	3PE	C3E-C3F-C3G-C3H
69	3X	106	3PE	C39-C3A-C3B-C3C
69	1L	701	3PE	O11-C1-C2-C3
69	1Y	210	3PE	O11-C1-C2-C3
69	1k	101	3PE	O11-C1-C2-C3
69	3C	503	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
69	3N	501	3PE	O11-C1-C2-C3
70	3X	104	PC1	O11-C1-C2-C3
75	3F	201	CDL	OB5-CB3-CB4-CB6
69	1L	702	3PE	C3F-C3G-C3H-C3I
69	1Y	213	3PE	C3D-C3E-C3F-C3G
69	1Y	215	3PE	C24-C25-C26-C27
75	4C	307	CDL	CA4-CA3-OA5-PA1
69	1m	201	3PE	C33-C34-C35-C36
70	1H	402	PC1	C24-C25-C26-C27
69	1f	104	3PE	C35-C36-C37-C38
69	3A	502	3PE	C24-C25-C26-C27
69	3X	101	3PE	C24-C25-C26-C27
75	3D	504	CDL	C52-C53-C54-C55
69	3C	515	3PE	C32-C31-O31-C3
70	1H	403	PC1	C32-C31-O31-C3
69	3G	111	3PE	O32-C31-O31-C3
69	3P	515	3PE	O32-C31-O31-C3
70	1Y	206	PC1	O32-C31-O31-C3
69	1d	206	3PE	C31-C32-C33-C34
69	3G	103	3PE	C21-C22-C23-C24
69	1L	712	3PE	C34-C35-C36-C37
69	3C	510	3PE	C29-C2A-C2B-C2C
69	3E	303	3PE	C29-C2A-C2B-C2C
75	1d	205	CDL	C15-C16-C17-C18
69	1g	203	3PE	O22-C21-O21-C2
69	1m	204	3PE	O22-C21-O21-C2
75	1q	202	CDL	OB7-CB5-OB6-CB4
75	3D	504	CDL	OB7-CB5-OB6-CB4
70	3J	106	PC1	C26-C27-C28-C29
69	3Y	105	3PE	O32-C31-O31-C3
70	1H	402	PC1	O32-C31-O31-C3
70	3P	509	PC1	O32-C31-O31-C3
69	3P	507	3PE	C25-C26-C27-C28
70	3X	104	PC1	C11-C12-N-C13
69	3E	303	3PE	C24-C25-C26-C27
69	1Y	213	3PE	C3-C2-O21-C21
69	1f	101	3PE	C3-C2-O21-C21
69	3C	510	3PE	C3-C2-O21-C21
69	3C	513	3PE	C1-C2-O21-C21
69	3G	102	3PE	C3-C2-O21-C21
69	3G	103	3PE	C1-C2-O21-C21
69	3G	111	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
69	3P	514	3PE	C1-C2-O21-C21
69	3W	103	3PE	C1-C2-O21-C21
75	1L	704	CDL	CB6-CB4-OB6-CB5
91	4C	303	PGV	C01-C02-O01-C1
69	3C	506	3PE	C38-C39-C3A-C3B
69	3P	520	3PE	C2C-C2D-C2E-C2F
69	1J	203	3PE	C32-C33-C34-C35
75	3N	502	CDL	C40-C41-C42-C43
69	3Q	503	3PE	C37-C38-C39-C3A
69	1L	705	3PE	C37-C38-C39-C3A
91	4J	101	PGV	O04-C19-O03-C01
69	3E	302	3PE	C32-C33-C34-C35
69	1Y	210	3PE	C25-C26-C27-C28
69	1Y	213	3PE	C24-C25-C26-C27
69	3R	305	3PE	C2D-C2E-C2F-C2G
70	1B	203	PC1	C35-C36-C37-C38
70	1Y	202	PC1	C23-C24-C25-C26
69	3G	101	3PE	O22-C21-O21-C2
69	1L	701	3PE	O11-C1-C2-O21
69	1Y	209	3PE	O11-C1-C2-O21
69	1g	203	3PE	O11-C1-C2-O21
69	1k	101	3PE	O11-C1-C2-O21
69	3C	503	3PE	O11-C1-C2-O21
69	3C	507	3PE	O11-C1-C2-O21
69	3N	501	3PE	O11-C1-C2-O21
69	3P	510	3PE	O11-C1-C2-O21
70	1h	203	PC1	O11-C1-C2-O21
70	3X	104	PC1	O11-C1-C2-O21
75	1H	401	CDL	OA5-CA3-CA4-OA6
75	1L	704	CDL	OA5-CA3-CA4-OA6
75	1L	704	CDL	OB5-CB3-CB4-OB6
75	1g	201	CDL	OB5-CB3-CB4-OB6
75	1q	202	CDL	OA5-CA3-CA4-OA6
69	1B	204	3PE	C33-C34-C35-C36
69	3Y	107	3PE	C2C-C2D-C2E-C2F
69	3E	302	3PE	C1-C2-C3-O31
69	3Q	502	3PE	C1-C2-C3-O31
69	3R	302	3PE	C1-C2-C3-O31
69	3X	101	3PE	C1-C2-C3-O31
75	1i	201	CDL	CB3-CB4-CB6-OB8
75	1q	202	CDL	CB3-CB4-CB6-OB8
69	1L	711	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
69	3R	304	3PE	C22-C21-O21-C2
87	4G	103	PEK	C2-C1-O01-C02
69	1L	710	3PE	C31-C32-C33-C34
75	3T	101	CDL	CA7-C31-C32-C33
85	3C	502	HEM	C4C-C3C-CAC-CBC
85	3P	501	HEM	C4B-C3B-CAB-CBB
69	3Y	104	3PE	C27-C28-C29-C2A
70	3R	303	PC1	C32-C33-C34-C35
69	1m	205	3PE	C3F-C3G-C3H-C3I
69	3W	102	3PE	C36-C37-C38-C39
69	1A	201	3PE	C28-C29-C2A-C2B
69	3R	302	3PE	C35-C36-C37-C38
82	1Y	203	PGT	C21-C22-C23-C24
69	1A	203	3PE	C12-C11-O13-P
69	1Y	213	3PE	C12-C11-O13-P
69	1o	201	3PE	C12-C11-O13-P
69	3G	105	3PE	C12-C11-O13-P
69	3J	102	3PE	C12-C11-O13-P
69	3Q	502	3PE	C12-C11-O13-P
69	3Q	503	3PE	C12-C11-O13-P
69	4G	101	3PE	C12-C11-O13-P
70	1A	202	PC1	C12-C11-O13-P
70	1H	404	PC1	C12-C11-O13-P
70	1J	202	PC1	C12-C11-O13-P
69	1Y	214	3PE	C33-C34-C35-C36
69	3Q	502	3PE	C26-C27-C28-C29
69	1M	502	3PE	O21-C2-C3-O31
69	3E	302	3PE	O21-C2-C3-O31
70	1H	404	PC1	O21-C2-C3-O31
75	1L	704	CDL	OB6-CB4-CB6-OB8
75	1d	205	CDL	OB6-CB4-CB6-OB8
69	3E	302	3PE	C3A-C3B-C3C-C3D
69	3P	505	3PE	C24-C25-C26-C27
69	3J	104	3PE	C33-C34-C35-C36
69	3G	105	3PE	C24-C25-C26-C27
69	3T	103	3PE	C3B-C3C-C3D-C3E
70	1B	202	PC1	C11-C12-N-C13
69	3A	502	3PE	C25-C26-C27-C28
69	3J	101	3PE	C23-C24-C25-C26
75	1L	704	CDL	C37-C38-C39-C40
69	1m	201	3PE	C3C-C3D-C3E-C3F
69	3C	506	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
69	3C	511	3PE	C36-C37-C38-C39
69	3A	503	3PE	C3D-C3E-C3F-C3G
69	1d	203	3PE	C39-C3A-C3B-C3C
69	1h	204	3PE	C32-C33-C34-C35
69	3C	511	3PE	C29-C2A-C2B-C2C
69	3P	511	3PE	C22-C23-C24-C25
69	3N	501	3PE	C2-C1-O11-P
69	3C	506	3PE	C26-C27-C28-C29
70	1B	203	PC1	O13-C11-C12-N
70	1H	404	PC1	O13-C11-C12-N
70	1J	202	PC1	O13-C11-C12-N
70	3T	102	PC1	O13-C11-C12-N
85	3C	501	HEM	C3D-CAD-CBD-CGD
69	1m	204	3PE	C3C-C3D-C3E-C3F
69	3J	101	3PE	C38-C39-C3A-C3B
69	3C	510	3PE	C23-C24-C25-C26
75	3A	501	CDL	CB7-C71-C72-C73
70	1H	403	PC1	O32-C31-O31-C3
69	1L	712	3PE	C26-C27-C28-C29
69	3C	509	3PE	C2C-C2D-C2E-C2F
69	3R	302	3PE	C3D-C3E-C3F-C3G
75	3N	502	CDL	C61-C62-C63-C64
91	4C	302	PGV	C25-C26-C27-C28
69	3P	516	3PE	C3A-C3B-C3C-C3D
91	4A	607	PGV	C7-C8-C9-C10
69	3D	502	3PE	C28-C29-C2A-C2B
75	3P	513	CDL	C72-C73-C74-C75
69	3P	506	3PE	C36-C37-C38-C39
69	1b	101	3PE	C23-C24-C25-C26
69	3A	503	3PE	C3E-C3F-C3G-C3H
69	3E	302	3PE	C2E-C2F-C2G-C2H
75	3A	501	CDL	C19-C20-C21-C22
75	3X	103	CDL	C82-C83-C84-C85
70	1B	202	PC1	C11-C12-N-C15
69	1L	711	3PE	C27-C28-C29-C2A
69	1L	702	3PE	C39-C3A-C3B-C3C
75	1Y	217	CDL	C55-C56-C57-C58
75	4C	306	CDL	C19-C20-C21-C22
75	1H	401	CDL	C51-C52-C53-C54
69	1B	204	3PE	C2E-C2F-C2G-C2H
69	3P	508	3PE	C2A-C2B-C2C-C2D
75	1L	704	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
69	1L	712	3PE	C36-C37-C38-C39
69	1N	401	3PE	O11-C1-C2-C3
69	1Y	209	3PE	O11-C1-C2-C3
69	3C	505	3PE	O11-C1-C2-C3
70	1B	203	PC1	O11-C1-C2-C3
70	1M	501	PC1	O11-C1-C2-C3
75	1H	401	CDL	OA5-CA3-CA4-CA6
75	1g	201	CDL	OA5-CA3-CA4-CA6
69	3R	304	3PE	O22-C21-O21-C2
69	3Y	105	3PE	O22-C21-O21-C2
87	4G	103	PEK	O02-C1-O01-C02
91	4G	102	PGV	O02-C1-O01-C02
69	1e	201	3PE	C2A-C2B-C2C-C2D
69	3J	101	3PE	C26-C27-C28-C29
69	3N	501	3PE	C22-C23-C24-C25
75	3P	513	CDL	C62-C63-C64-C65
73	1F	501	FMN	N10-C1'-C2'-O2'
75	1d	205	CDL	C54-C55-C56-C57
69	1L	705	3PE	C33-C34-C35-C36
87	4G	103	PEK	C26-C27-C28-C29
69	1L	710	3PE	C32-C33-C34-C35
69	3A	502	3PE	C2C-C2D-C2E-C2F
69	3C	508	3PE	C23-C24-C25-C26
70	3P	509	PC1	C3D-C3E-C3F-C3G
70	1B	202	PC1	C32-C31-O31-C3
75	1L	704	CDL	C31-CA7-OA8-CA6
69	3A	503	3PE	C26-C27-C28-C29
69	3Y	101	3PE	C2E-C2F-C2G-C2H
69	3A	502	3PE	C39-C3A-C3B-C3C
69	3C	515	3PE	O32-C31-O31-C3
70	1B	202	PC1	O32-C31-O31-C3
69	1l	204	3PE	C2-C1-O11-P
69	3P	516	3PE	C2-C1-O11-P
75	3N	502	CDL	CB4-CB3-OB5-PB2
91	4A	608	PGV	C02-C03-O11-P
91	4C	304	PGV	C05-C04-O12-P
91	4K	101	PGV	C02-C03-O11-P
70	3X	104	PC1	C2A-C2B-C2C-C2D
81	1n	201	EHZ	C11-C10-S1-C9
75	1g	201	CDL	C22-C23-C24-C25
75	3F	201	CDL	C59-C60-C61-C62
69	1B	204	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
69	1Y	214	3PE	C39-C3A-C3B-C3C
69	1l	204	3PE	C3D-C3E-C3F-C3G
69	1m	201	3PE	C2D-C2E-C2F-C2G
69	1N	401	3PE	O11-C1-C2-O21
69	1d	201	3PE	O11-C1-C2-O21
69	3P	503	3PE	O11-C1-C2-O21
70	1B	203	PC1	O11-C1-C2-O21
75	3F	201	CDL	OB5-CB3-CB4-OB6
75	3X	103	CDL	OB5-CB3-CB4-OB6
75	3Y	106	CDL	OB5-CB3-CB4-OB6
69	3G	109	3PE	C32-C33-C34-C35
69	1g	203	3PE	C34-C35-C36-C37
70	1Y	207	PC1	C3C-C3D-C3E-C3F
91	4G	102	PGV	C2-C1-O01-C02
70	3R	303	PC1	C11-C12-N-C14
69	3C	515	3PE	C28-C29-C2A-C2B
75	3P	513	CDL	C20-C21-C22-C23
69	1l	204	3PE	C27-C28-C29-C2A
69	3C	510	3PE	C25-C26-C27-C28
69	3J	104	3PE	C2B-C2C-C2D-C2E
75	1d	202	CDL	C58-C59-C60-C61
69	3N	503	3PE	C34-C35-C36-C37
69	1L	708	3PE	O21-C2-C3-O31
69	1d	203	3PE	O21-C2-C3-O31
69	1f	101	3PE	O21-C2-C3-O31
69	3P	505	3PE	O21-C2-C3-O31
69	3Y	104	3PE	O21-C2-C3-O31
70	1B	203	PC1	O21-C2-C3-O31
75	1i	201	CDL	OB6-CB4-CB6-OB8
69	3W	103	3PE	C27-C28-C29-C2A
69	1J	201	3PE	C2A-C2B-C2C-C2D
69	1L	705	3PE	C28-C29-C2A-C2B
69	1Y	208	3PE	C23-C24-C25-C26
69	1N	401	3PE	C33-C34-C35-C36
69	1Y	210	3PE	C1-C2-C3-O31
69	1k	101	3PE	C1-C2-C3-O31
69	1l	202	3PE	C1-C2-C3-O31
69	3P	505	3PE	C1-C2-C3-O31
69	3P	506	3PE	C1-C2-C3-O31
69	3P	517	3PE	C1-C2-C3-O31
69	3W	103	3PE	C1-C2-C3-O31
75	1N	402	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
75	1g	201	CDL	CA3-CA4-CA6-OA8
81	1T	101	EHZ	C10-C11-N1-C12
81	1n	201	EHZ	C10-C11-N1-C12
75	4C	306	CDL	C54-C55-C56-C57
70	1h	202	PC1	C29-C2A-C2B-C2C
75	4B	302	CDL	C13-C14-C15-C16
75	1N	402	CDL	C54-C55-C56-C57
69	3C	506	3PE	C36-C37-C38-C39
75	1q	202	CDL	C19-C20-C21-C22
91	4C	304	PGV	C4-C5-C6-C7
75	4C	307	CDL	CB4-CB6-OB8-CB7
69	3G	106	3PE	C33-C34-C35-C36
69	3P	519	3PE	C28-C29-C2A-C2B
69	3Y	104	3PE	C25-C26-C27-C28
75	1L	704	CDL	OA9-CA7-OA8-CA6
69	3P	510	3PE	C32-C33-C34-C35
69	3X	105	3PE	C3E-C3F-C3G-C3H
69	3E	302	3PE	C23-C24-C25-C26
75	3N	502	CDL	C55-C56-C57-C58
69	3E	303	3PE	C32-C33-C34-C35
75	3Y	106	CDL	C81-C82-C83-C84
79	1P	501	NDP	O4D-C4D-C5D-O5D
75	1d	202	CDL	C32-C33-C34-C35
75	1d	205	CDL	C62-C63-C64-C65
69	1B	204	3PE	C1-O11-P-O12
69	1B	205	3PE	C1-O11-P-O12
69	1J	201	3PE	C11-O13-P-O11
69	1J	201	3PE	C11-O13-P-O12
69	1J	201	3PE	C11-O13-P-O14
69	1L	703	3PE	C1-O11-P-O13
69	1L	703	3PE	C1-O11-P-O14
69	1L	706	3PE	C11-O13-P-O14
69	1L	707	3PE	C1-O11-P-O14
69	1L	708	3PE	C1-O11-P-O12
69	1L	708	3PE	C1-O11-P-O13
69	1L	709	3PE	C1-O11-P-O14
69	1L	709	3PE	C11-O13-P-O14
69	1L	710	3PE	C1-O11-P-O14
69	1L	712	3PE	C1-O11-P-O14
69	1M	502	3PE	C1-O11-P-O14
69	1M	502	3PE	C11-O13-P-O11
69	1M	502	3PE	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
69	1Y	205	3PE	C11-O13-P-O11
69	1Y	205	3PE	C11-O13-P-O12
69	1Y	209	3PE	C1-O11-P-O14
69	1Y	210	3PE	C1-O11-P-O14
69	1Y	211	3PE	C11-O13-P-O11
69	1Y	211	3PE	C11-O13-P-O14
69	1Y	212	3PE	C1-O11-P-O12
69	1Y	212	3PE	C1-O11-P-O13
69	1Y	213	3PE	C1-O11-P-O12
69	1Y	215	3PE	C1-O11-P-O12
69	1Y	215	3PE	C11-O13-P-O11
69	1Y	215	3PE	C11-O13-P-O12
69	1Y	215	3PE	C11-O13-P-O14
69	1d	201	3PE	O13-C11-C12-N
69	1e	201	3PE	C1-O11-P-O13
69	1e	201	3PE	C11-O13-P-O12
69	1f	101	3PE	C1-O11-P-O13
69	1f	101	3PE	C1-O11-P-O14
69	1f	101	3PE	C11-O13-P-O12
69	1f	101	3PE	O13-C11-C12-N
69	1f	102	3PE	C11-O13-P-O11
69	1f	104	3PE	C1-O11-P-O14
69	1f	104	3PE	C11-O13-P-O11
69	1g	203	3PE	C1-O11-P-O14
69	1k	101	3PE	C1-O11-P-O14
69	1l	203	3PE	C11-O13-P-O12
69	1m	201	3PE	C1-O11-P-O14
69	1m	204	3PE	C1-O11-P-O13
69	1m	204	3PE	C1-O11-P-O14
69	1m	204	3PE	C11-O13-P-O14
69	1m	205	3PE	C11-O13-P-O14
69	1o	201	3PE	O13-C11-C12-N
69	3A	502	3PE	C11-O13-P-O14
69	3C	503	3PE	C11-O13-P-O11
69	3C	503	3PE	C11-O13-P-O14
69	3C	505	3PE	C1-O11-P-O14
69	3C	506	3PE	C1-O11-P-O12
69	3C	506	3PE	C1-O11-P-O13
69	3C	506	3PE	C11-O13-P-O14
69	3C	509	3PE	C1-O11-P-O14
69	3C	510	3PE	C1-O11-P-O12
69	3C	510	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
69	3C	511	3PE	C1-O11-P-O14
69	3C	512	3PE	C1-O11-P-O12
69	3C	512	3PE	C1-O11-P-O13
69	3C	512	3PE	C1-O11-P-O14
69	3C	513	3PE	C1-O11-P-O14
69	3C	514	3PE	C1-O11-P-O14
69	3C	515	3PE	C11-O13-P-O11
69	3C	515	3PE	C11-O13-P-O12
69	3C	516	3PE	C11-O13-P-O12
69	3C	517	3PE	C1-O11-P-O14
69	3D	502	3PE	C1-O11-P-O14
69	3D	503	3PE	C1-O11-P-O14
69	3D	503	3PE	C11-O13-P-O14
69	3E	302	3PE	C1-O11-P-O14
69	3E	303	3PE	C1-O11-P-O12
69	3E	303	3PE	C1-O11-P-O13
69	3E	303	3PE	C11-O13-P-O11
69	3E	303	3PE	C11-O13-P-O12
69	3E	303	3PE	C11-O13-P-O14
69	3E	303	3PE	O13-C11-C12-N
69	3G	102	3PE	C1-O11-P-O14
69	3G	103	3PE	C1-O11-P-O12
69	3G	103	3PE	C1-O11-P-O13
69	3G	103	3PE	C1-O11-P-O14
69	3G	104	3PE	C1-O11-P-O12
69	3G	106	3PE	C1-O11-P-O12
69	3G	107	3PE	C1-O11-P-O14
69	3G	108	3PE	C1-O11-P-O12
69	3G	110	3PE	C1-O11-P-O13
69	3G	111	3PE	C11-O13-P-O11
69	3J	101	3PE	C11-O13-P-O14
69	3J	102	3PE	C1-O11-P-O14
69	3J	102	3PE	C11-O13-P-O14
69	3J	103	3PE	C1-O11-P-O12
69	3J	104	3PE	C1-O11-P-O12
69	3J	105	3PE	C11-O13-P-O11
69	3N	501	3PE	C1-O11-P-O13
69	3N	501	3PE	C11-O13-P-O11
69	3N	503	3PE	C1-O11-P-O13
69	3N	503	3PE	C11-O13-P-O14
69	3P	503	3PE	C1-O11-P-O12
69	3P	504	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
69	3P	505	3PE	C1-O11-P-O14
69	3P	507	3PE	C1-O11-P-O13
69	3P	508	3PE	C11-O13-P-O14
69	3P	510	3PE	C1-O11-P-O12
69	3P	512	3PE	C1-O11-P-O14
69	3P	515	3PE	C1-O11-P-O12
69	3P	515	3PE	O13-C11-C12-N
69	3P	517	3PE	C11-O13-P-O14
69	3P	519	3PE	C1-O11-P-O12
69	3P	519	3PE	C1-O11-P-O13
69	3P	519	3PE	C1-O11-P-O14
69	3P	520	3PE	C1-O11-P-O12
69	3P	520	3PE	C1-O11-P-O13
69	3P	520	3PE	O13-C11-C12-N
69	3Q	504	3PE	C1-O11-P-O12
69	3Q	504	3PE	C1-O11-P-O13
69	3Q	504	3PE	C1-O11-P-O14
69	3Q	504	3PE	C11-O13-P-O12
69	3R	304	3PE	C1-O11-P-O12
69	3R	304	3PE	C1-O11-P-O13
69	3R	304	3PE	C1-O11-P-O14
69	3S	201	3PE	C11-O13-P-O11
69	3S	201	3PE	C11-O13-P-O14
69	3T	103	3PE	C1-O11-P-O14
69	3T	103	3PE	C11-O13-P-O14
69	3W	102	3PE	C1-O11-P-O13
69	3W	102	3PE	C11-O13-P-O12
69	3X	101	3PE	C1-O11-P-O12
69	3X	106	3PE	C1-O11-P-O12
69	3X	108	3PE	C11-O13-P-O11
69	3X	108	3PE	C11-O13-P-O12
69	3X	108	3PE	C11-O13-P-O14
69	3Y	104	3PE	C11-O13-P-O11
69	3Y	104	3PE	C11-O13-P-O12
69	3Y	104	3PE	C11-O13-P-O14
69	3Y	107	3PE	C1-O11-P-O12
69	3Y	107	3PE	C1-O11-P-O13
69	3Y	107	3PE	C11-O13-P-O11
69	3Y	107	3PE	C11-O13-P-O12
69	4G	101	3PE	C1-O11-P-O13
69	4G	101	3PE	C11-O13-P-O14
70	1B	202	PC1	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
70	1B	203	PC1	C11-O13-P-O12
70	1H	403	PC1	C1-O11-P-O14
70	1H	404	PC1	C11-O13-P-O14
70	1J	202	PC1	C11-O13-P-O11
70	1M	501	PC1	C11-O13-P-O12
70	1M	501	PC1	C1-O11-P-O13
70	1Y	202	PC1	C11-O13-P-O11
70	1d	204	PC1	C1-O11-P-O12
70	1h	203	PC1	C11-O13-P-O14
70	3J	106	PC1	C1-O11-P-O12
70	3P	509	PC1	C11-O13-P-O14
70	3P	509	PC1	C11-C12-N-C13
70	3R	303	PC1	C11-O13-P-O14
70	3T	102	PC1	C11-O13-P-O14
70	3T	102	PC1	C1-O11-P-O14
75	1L	704	CDL	CA2-OA2-PA1-OA3
75	1L	704	CDL	CB2-OB2-PB2-OB3
75	1L	704	CDL	CB3-OB5-PB2-OB4
75	1N	402	CDL	CA2-OA2-PA1-OA3
75	1N	402	CDL	CA3-OA5-PA1-OA3
75	1N	402	CDL	CB2-OB2-PB2-OB3
75	1N	402	CDL	CB2-OB2-PB2-OB5
75	1d	202	CDL	CA2-OA2-PA1-OA5
75	1d	202	CDL	CA3-OA5-PA1-OA3
75	1d	202	CDL	CB2-OB2-PB2-OB4
75	1d	205	CDL	CA2-OA2-PA1-OA3
75	1d	205	CDL	CA2-OA2-PA1-OA4
75	1d	205	CDL	CA2-OA2-PA1-OA5
75	1d	205	CDL	CA3-OA5-PA1-OA4
75	1d	205	CDL	CB3-OB5-PB2-OB2
75	1d	205	CDL	CB3-OB5-PB2-OB4
75	1g	201	CDL	CB3-OB5-PB2-OB3
75	1q	201	CDL	CA2-OA2-PA1-OA3
75	1q	201	CDL	CA2-OA2-PA1-OA5
75	1q	202	CDL	CA3-OA5-PA1-OA3
75	3A	501	CDL	CB2-OB2-PB2-OB4
75	3D	504	CDL	CA3-OA5-PA1-OA2
75	3D	504	CDL	CA3-OA5-PA1-OA3
75	3D	504	CDL	CA3-OA5-PA1-OA4
75	3D	504	CDL	CB2-OB2-PB2-OB4
75	3F	201	CDL	CA2-OA2-PA1-OA3
75	3F	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
75	3N	502	CDL	CA3-OA5-PA1-OA3
75	3N	502	CDL	CB2-OB2-PB2-OB5
75	3N	502	CDL	CB3-OB5-PB2-OB3
75	3P	513	CDL	CA2-OA2-PA1-OA3
75	3X	103	CDL	CA3-OA5-PA1-OA4
75	3X	103	CDL	CB3-OB5-PB2-OB2
75	3Y	106	CDL	CA2-OA2-PA1-OA3
75	3Y	106	CDL	CA3-OA5-PA1-OA2
75	4B	302	CDL	CA2-OA2-PA1-OA3
75	4B	302	CDL	CB2-OB2-PB2-OB3
75	4C	306	CDL	CA2-OA2-PA1-OA3
75	4C	307	CDL	CB2-OB2-PB2-OB3
82	1Y	203	PGT	C1-O3P-P-O4P
82	1Y	203	PGT	C4-O4P-P-O3P
82	1Y	203	PGT	C4-O4P-P-O1P
87	3X	102	PEK	C04-O12-P-O11
87	3X	102	PEK	C04-O12-P-O13
91	4A	606	PGV	C03-O11-P-O13
91	4A	607	PGV	C04-O12-P-O14
91	4A	609	PGV	C03-O11-P-O14
91	4A	609	PGV	C04-O12-P-O13
91	4C	303	PGV	C04-O12-P-O13
91	4C	305	PGV	C03-O11-P-O13
91	4G	102	PGV	C04-O12-P-O11
91	4J	101	PGV	C03-O11-P-O14
91	4J	101	PGV	C04-O12-P-O13
91	4K	101	PGV	C03-O11-P-O14
91	4K	101	PGV	C04-O12-P-O11
93	4B	303	PSC	C03-O11-P-O12
93	4B	303	PSC	C04-O12-P-O11
69	1L	701	3PE	C32-C33-C34-C35
69	3P	514	3PE	C34-C35-C36-C37
75	1N	402	CDL	C77-C78-C79-C80
69	1Z	201	3PE	C32-C33-C34-C35
70	1B	203	PC1	C28-C29-C2A-C2B
69	3P	518	3PE	C2C-C2D-C2E-C2F
69	3X	107	3PE	C36-C37-C38-C39
69	1A	203	3PE	C2-C1-O11-P
69	1L	711	3PE	C2-C1-O11-P
69	1Y	201	3PE	C2-C1-O11-P
69	1Y	209	3PE	C2-C1-O11-P
69	1Y	210	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
69	1l	203	3PE	C2-C1-O11-P
69	3A	503	3PE	C2-C1-O11-P
69	3C	504	3PE	C2-C1-O11-P
69	3C	511	3PE	C2-C1-O11-P
69	3G	108	3PE	C2-C1-O11-P
69	3N	503	3PE	C2-C1-O11-P
69	3P	506	3PE	C2-C1-O11-P
69	3P	507	3PE	C2-C1-O11-P
69	4G	101	3PE	C2-C1-O11-P
73	1F	501	FMN	C4'-C5'-O5'-P
75	1g	201	CDL	CA4-CA3-OA5-PA1
75	3F	201	CDL	CB4-CB3-OB5-PB2
75	4C	306	CDL	CA4-CA3-OA5-PA1
82	1Y	203	PGT	C5-C4-O4P-P
91	4A	607	PGV	C02-C03-O11-P
91	4C	303	PGV	C02-C03-O11-P
91	4G	102	PGV	C05-C04-O12-P
91	4N	101	PGV	C02-C03-O11-P
69	1Y	214	3PE	C3B-C3C-C3D-C3E
69	1o	201	3PE	C28-C29-C2A-C2B
69	1g	202	3PE	C2B-C2C-C2D-C2E
69	1l	202	3PE	C31-C32-C33-C34
69	3C	512	3PE	C38-C39-C3A-C3B
75	4C	306	CDL	C22-C23-C24-C25
69	1N	401	3PE	C3E-C3F-C3G-C3H
69	1Y	213	3PE	C2E-C2F-C2G-C2H
69	3P	515	3PE	C22-C23-C24-C25
69	3X	101	3PE	C3E-C3F-C3G-C3H
75	3A	501	CDL	C78-C79-C80-C81
69	3J	103	3PE	C3E-C3F-C3G-C3H
69	1e	201	3PE	C31-C32-C33-C34
69	3A	503	3PE	C31-C32-C33-C34
70	3T	102	PC1	C31-C32-C33-C34
70	3T	102	PC1	C3C-C3D-C3E-C3F
70	3R	303	PC1	C39-C3A-C3B-C3C
69	1A	203	3PE	C29-C2A-C2B-C2C
69	1B	204	3PE	C27-C28-C29-C2A
69	3A	502	3PE	C3B-C3C-C3D-C3E
69	1J	203	3PE	C23-C24-C25-C26
69	3W	103	3PE	C39-C3A-C3B-C3C
69	1L	703	3PE	C3-C2-O21-C21
69	1L	710	3PE	C1-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
69	1Y	205	3PE	C3-C2-O21-C21
69	1Y	209	3PE	C1-C2-O21-C21
69	1g	203	3PE	C1-C2-O21-C21
69	1h	204	3PE	C3-C2-O21-C21
69	1l	202	3PE	C3-C2-O21-C21
69	1l	204	3PE	C3-C2-O21-C21
69	1m	202	3PE	C1-C2-O21-C21
69	3Q	503	3PE	C1-C2-O21-C21
69	3W	101	3PE	C3-C2-O21-C21
69	3Y	101	3PE	C3-C2-O21-C21
70	1d	204	PC1	C1-C2-O21-C21
75	1d	205	CDL	CB3-CB4-OB6-CB5
75	1g	201	CDL	CA6-CA4-OA6-CA5
75	3N	502	CDL	CB6-CB4-OB6-CB5
69	1M	502	3PE	C2B-C2C-C2D-C2E
69	1Y	215	3PE	C29-C2A-C2B-C2C
75	1d	202	CDL	C23-C24-C25-C26
69	3R	305	3PE	C34-C35-C36-C37
75	3X	103	CDL	C12-C13-C14-C15
91	4C	305	PGV	C6-C7-C8-C9
69	1l	204	3PE	C28-C29-C2A-C2B
69	3C	505	3PE	C34-C35-C36-C37
69	3Q	503	3PE	C2E-C2F-C2G-C2H
70	1P	502	PC1	C11-C12-N-C15
70	3R	303	PC1	C11-C12-N-C13
69	1d	201	3PE	O11-C1-C2-C3
69	3C	507	3PE	O11-C1-C2-C3
69	3G	101	3PE	O11-C1-C2-C3
69	3P	503	3PE	O11-C1-C2-C3
69	3P	514	3PE	O11-C1-C2-C3
69	1L	702	3PE	C3A-C3B-C3C-C3D
69	1L	705	3PE	C2E-C2F-C2G-C2H
69	3Y	101	3PE	C33-C34-C35-C36
69	1m	203	3PE	C2B-C2C-C2D-C2E
70	1d	204	PC1	C2-C3-O31-C31
69	3X	108	3PE	C3C-C3D-C3E-C3F
91	4A	609	PGV	C9-C10-C11-C12
91	4A	609	PGV	C11-C12-C13-C14
91	4C	305	PGV	C11-C12-C13-C14
75	1L	704	CDL	CA5-C11-C12-C13
75	1d	202	CDL	CB5-C51-C52-C53
69	3C	505	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
69	3G	101	3PE	O11-C1-C2-O21
70	1H	403	PC1	O11-C1-C2-O21
69	1m	202	3PE	C2A-C2B-C2C-C2D
75	4C	307	CDL	C15-C16-C17-C18
69	3G	110	3PE	C29-C2A-C2B-C2C
69	3J	105	3PE	C29-C2A-C2B-C2C
69	1Y	208	3PE	O32-C31-O31-C3
69	1L	707	3PE	C34-C35-C36-C37
69	3A	503	3PE	C3A-C3B-C3C-C3D
69	3R	304	3PE	C3B-C3C-C3D-C3E
81	1T	101	EHZ	C21-C22-C23-C24
91	4C	305	PGV	C7-C8-C9-C10
69	1Y	213	3PE	C25-C26-C27-C28
69	1d	203	3PE	C38-C39-C3A-C3B
69	3C	507	3PE	C36-C37-C38-C39
69	3P	519	3PE	C38-C39-C3A-C3B
69	1d	201	3PE	C3A-C3B-C3C-C3D
75	1d	202	CDL	C39-C40-C41-C42
69	1g	202	3PE	C3C-C3D-C3E-C3F
69	1L	710	3PE	C2-C1-O11-P
75	4C	307	CDL	CB4-CB3-OB5-PB2
69	1Y	201	3PE	C34-C35-C36-C37
69	3N	501	3PE	C34-C35-C36-C37
87	4G	103	PEK	C28-C29-C30-C31
69	1L	705	3PE	O21-C2-C3-O31
69	1Y	209	3PE	O21-C2-C3-O31
75	3Y	106	CDL	OB6-CB4-CB6-OB8
75	3D	504	CDL	C11-C12-C13-C14
75	3F	201	CDL	C19-C20-C21-C22
69	1M	502	3PE	C3A-C3B-C3C-C3D
69	3A	503	3PE	C22-C23-C24-C25
69	3P	512	3PE	C35-C36-C37-C38
69	3R	305	3PE	C32-C33-C34-C35
70	1H	402	PC1	C2A-C2B-C2C-C2D
69	3R	302	3PE	C33-C34-C35-C36
70	1h	203	PC1	C23-C24-C25-C26
70	1B	202	PC1	C11-C12-N-C14
88	4A	601	HEA	C4D-C3D-CAD-CBD
69	3C	507	3PE	C32-C33-C34-C35
69	3X	106	3PE	C33-C34-C35-C36
75	1Y	217	CDL	OB7-CB5-OB6-CB4
75	3X	103	CDL	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
69	1Z	201	3PE	C24-C25-C26-C27
91	4G	102	PGV	C26-C27-C28-C29
69	3R	304	3PE	C31-C32-C33-C34
69	1b	101	3PE	C29-C2A-C2B-C2C
69	1d	201	3PE	C3B-C3C-C3D-C3E
69	3G	102	3PE	C22-C23-C24-C25
75	3Y	106	CDL	C78-C79-C80-C81
75	1g	201	CDL	C56-C57-C58-C59
69	4G	104	3PE	C2A-C2B-C2C-C2D
69	3D	502	3PE	C32-C33-C34-C35
91	4A	606	PGV	C11-C12-C13-C14
91	4A	607	PGV	C9-C10-C11-C12
69	1Y	208	3PE	C32-C31-O31-C3
69	3X	101	3PE	C25-C26-C27-C28
69	1L	710	3PE	C38-C39-C3A-C3B
69	3W	101	3PE	C37-C38-C39-C3A
69	3G	109	3PE	C31-C32-C33-C34
69	3D	503	3PE	C27-C28-C29-C2A
69	3G	111	3PE	C34-C35-C36-C37
75	3X	103	CDL	C22-C23-C24-C25
75	4C	306	CDL	C58-C59-C60-C61
69	3J	101	3PE	C2C-C2D-C2E-C2F
69	3C	511	3PE	C38-C39-C3A-C3B
69	3P	518	3PE	C2E-C2F-C2G-C2H
75	1q	202	CDL	C38-C39-C40-C41
69	3P	503	3PE	C2C-C2D-C2E-C2F
69	3C	504	3PE	C24-C25-C26-C27
69	3S	201	3PE	C29-C2A-C2B-C2C
69	1m	203	3PE	C21-C22-C23-C24
69	1B	204	3PE	C3D-C3E-C3F-C3G
69	3G	101	3PE	C2C-C2D-C2E-C2F
69	3X	107	3PE	C28-C29-C2A-C2B
69	3C	503	3PE	C2-C1-O11-P
69	3R	304	3PE	C2-C1-O11-P
75	1d	202	CDL	C12-C13-C14-C15
69	1Y	209	3PE	C33-C34-C35-C36
69	3C	507	3PE	C29-C2A-C2B-C2C
69	1J	203	3PE	C32-C31-O31-C3
75	1Y	217	CDL	C31-CA7-OA8-CA6
70	1J	202	PC1	C33-C34-C35-C36
69	1Y	215	3PE	O11-C1-C2-O21
69	1l	203	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
75	1d	205	CDL	OB5-CB3-CB4-OB6
69	3D	502	3PE	C33-C34-C35-C36
69	3Q	504	3PE	C32-C33-C34-C35
75	1Y	217	CDL	OA9-CA7-OA8-CA6
69	3P	515	3PE	C2D-C2E-C2F-C2G
69	3P	516	3PE	C22-C23-C24-C25
75	1i	201	CDL	C59-C60-C61-C62
69	3C	505	3PE	C32-C33-C34-C35
70	1d	204	PC1	C3C-C3D-C3E-C3F
69	3P	519	3PE	C2A-C2B-C2C-C2D
69	3W	101	3PE	C39-C3A-C3B-C3C
70	1h	202	PC1	C2B-C2C-C2D-C2E
69	1l	202	3PE	C37-C38-C39-C3A
75	1g	201	CDL	C76-C77-C78-C79
75	3N	502	CDL	C32-C33-C34-C35
69	1h	204	3PE	C22-C23-C24-C25
69	3G	107	3PE	C25-C26-C27-C28
69	3J	105	3PE	C3E-C3F-C3G-C3H
82	1Y	203	PGT	C14-C15-C16-C17
93	4B	303	PSC	C12-C13-C14-C15
69	3X	101	3PE	C31-C32-C33-C34
69	3X	108	3PE	C3A-C3B-C3C-C3D
69	3Y	107	3PE	C34-C35-C36-C37
75	4B	302	CDL	C16-C17-C18-C19
75	4C	306	CDL	C14-C15-C16-C17
69	3C	507	3PE	O21-C2-C3-O31
69	3G	111	3PE	O21-C2-C3-O31
75	1d	205	CDL	OA6-CA4-CA6-OA8
91	4C	301	PGV	C11-C10-C9-C8
69	3C	504	3PE	C35-C36-C37-C38
69	3Q	503	3PE	C34-C35-C36-C37
70	1H	404	PC1	C34-C35-C36-C37
75	1Y	217	CDL	C82-C83-C84-C85
75	3F	201	CDL	C39-C40-C41-C42
70	1P	502	PC1	C22-C23-C24-C25
75	3N	502	CDL	C31-C32-C33-C34
69	1b	101	3PE	C2B-C2C-C2D-C2E
69	1d	201	3PE	C2D-C2E-C2F-C2G
69	3E	303	3PE	C37-C38-C39-C3A
70	3R	303	PC1	C23-C24-C25-C26
82	1Y	203	PGT	C36-C37-C38-C39
88	4A	601	HEA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
69	3C	513	3PE	C24-C25-C26-C27
69	3G	106	3PE	C32-C33-C34-C35
69	1Y	213	3PE	C28-C29-C2A-C2B
81	1T	101	EHZ	C1-C21-C22-C23
69	3D	502	3PE	C2-C3-O31-C31
75	3P	513	CDL	C83-C84-C85-C86
91	4K	101	PGV	C24-C25-C26-C27
69	1M	502	3PE	C32-C33-C34-C35
69	3P	514	3PE	C38-C39-C3A-C3B
69	3X	106	3PE	C32-C33-C34-C35
75	1d	205	CDL	C57-C58-C59-C60
75	4B	302	CDL	C78-C79-C80-C81
69	1Y	215	3PE	C38-C39-C3A-C3B
69	3Q	503	3PE	C38-C39-C3A-C3B
70	1h	202	PC1	C26-C27-C28-C29
69	3Q	504	3PE	C2-C1-O11-P
69	3Y	102	3PE	C2-C1-O11-P
75	1N	402	CDL	C1-CB2-OB2-PB2
75	1d	202	CDL	CA4-CA3-OA5-PA1
69	3C	509	3PE	C31-C32-C33-C34
75	3F	201	CDL	C62-C63-C64-C65
75	3X	103	CDL	C15-C16-C17-C18
88	4A	601	HEA	C2D-C3D-CAD-CBD
69	1L	703	3PE	C2D-C2E-C2F-C2G
69	1L	709	3PE	C36-C37-C38-C39
69	1f	103	3PE	C33-C34-C35-C36
69	3X	107	3PE	C3E-C3F-C3G-C3H
75	3N	502	CDL	C15-C16-C17-C18
69	1M	502	3PE	C1-C2-C3-O31
69	1g	202	3PE	C1-C2-C3-O31
75	3A	501	CDL	CA3-CA4-CA6-OA8
75	3X	103	CDL	C78-C79-C80-C81
69	1d	203	3PE	C29-C2A-C2B-C2C
69	3P	510	3PE	C36-C37-C38-C39
75	1L	704	CDL	C82-C83-C84-C85
69	1m	204	3PE	C2A-C2B-C2C-C2D
69	3Y	107	3PE	C35-C36-C37-C38
75	1q	202	CDL	C62-C63-C64-C65
69	3C	508	3PE	C21-C22-C23-C24
69	3G	102	3PE	C31-C32-C33-C34
69	3E	302	3PE	C38-C39-C3A-C3B
70	3X	104	PC1	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
75	1L	704	CDL	C55-C56-C57-C58
69	1k	101	3PE	C3C-C3D-C3E-C3F
69	1L	706	3PE	C3-C2-O21-C21
69	1L	708	3PE	C3-C2-O21-C21
69	3J	103	3PE	C1-C2-O21-C21
69	3Q	504	3PE	C1-C2-O21-C21
75	3X	103	CDL	CB6-CB4-OB6-CB5
76	1I	203	AYA	C-CA-N-CT
69	3G	110	3PE	C32-C33-C34-C35
75	3A	501	CDL	C40-C41-C42-C43
69	3E	302	3PE	C34-C35-C36-C37
69	1L	712	3PE	C3A-C3B-C3C-C3D
69	1m	205	3PE	C3A-C3B-C3C-C3D
69	3A	503	3PE	C28-C29-C2A-C2B
75	3A	501	CDL	C14-C15-C16-C17
82	1Y	203	PGT	C17-C18-C19-C20
69	3C	509	3PE	C2D-C2E-C2F-C2G
69	3N	503	3PE	C22-C23-C24-C25
85	3P	501	HEM	CAA-CBA-CGA-O2A
69	3C	513	3PE	C2B-C2C-C2D-C2E
69	1h	204	3PE	C3D-C3E-C3F-C3G
70	1h	202	PC1	C24-C25-C26-C27
70	3R	303	PC1	C11-C12-N-C15
69	3C	505	3PE	C26-C27-C28-C29
69	1o	201	3PE	C27-C28-C29-C2A
91	4A	607	PGV	C20-C21-C22-C23
69	3G	111	3PE	O11-C1-C2-O21
69	3N	503	3PE	O11-C1-C2-O21
69	3P	519	3PE	O11-C1-C2-O21
69	3G	111	3PE	C25-C26-C27-C28
70	3R	303	PC1	C29-C2A-C2B-C2C
69	1l	204	3PE	C23-C24-C25-C26
85	3P	502	HEM	CAA-CBA-CGA-O2A
69	3A	502	3PE	C33-C34-C35-C36
69	3C	506	3PE	C33-C34-C35-C36
69	3Y	105	3PE	C33-C34-C35-C36
69	3P	516	3PE	C28-C29-C2A-C2B
69	3P	510	3PE	C2-C1-O11-P
69	4G	104	3PE	C2-C1-O11-P
70	1Y	207	PC1	C2-C1-O11-P
75	1d	202	CDL	CB4-CB3-OB5-PB2
77	1O	401	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
82	1Y	203	PGT	C2-C1-O3P-P
91	4C	305	PGV	C05-C04-O12-P
69	3P	507	3PE	C35-C36-C37-C38
75	4C	306	CDL	OB5-CB3-CB4-CB6
69	3W	102	3PE	C37-C38-C39-C3A
75	3N	502	CDL	C37-C38-C39-C40
85	3P	501	HEM	CAA-CBA-CGA-O1A
85	3P	502	HEM	CAA-CBA-CGA-O1A
69	1d	201	3PE	C2B-C2C-C2D-C2E
69	3P	503	3PE	C26-C27-C28-C29
69	3P	520	3PE	C35-C36-C37-C38
91	4A	608	PGV	C9-C10-C11-C12
85	3C	502	HEM	CAA-CBA-CGA-O1A
85	3C	502	HEM	CAA-CBA-CGA-O2A
85	3P	501	HEM	CAD-CBD-CGD-O2D
88	4A	601	HEA	CAD-CBD-CGD-O2D
69	1f	103	3PE	C37-C38-C39-C3A
70	1Y	207	PC1	C25-C26-C27-C28
75	3T	101	CDL	C52-C53-C54-C55
75	3D	504	CDL	C54-C55-C56-C57
79	1P	501	NDP	C2N-C3N-C7N-N7N
87	3X	102	PEK	C5-C6-C7-C8
69	1d	203	3PE	C22-C23-C24-C25
75	4C	306	CDL	C11-C12-C13-C14
85	3C	501	HEM	CAA-CBA-CGA-O1A
85	3C	501	HEM	CAA-CBA-CGA-O2A
85	3P	501	HEM	CAD-CBD-CGD-O1D
69	1L	712	3PE	C2E-C2F-C2G-C2H
69	3C	513	3PE	C28-C29-C2A-C2B
69	3P	507	3PE	C2B-C2C-C2D-C2E
69	3Y	104	3PE	C2B-C2C-C2D-C2E
75	3F	201	CDL	C72-C73-C74-C75
69	1L	701	3PE	C2E-C2F-C2G-C2H
69	1d	203	3PE	C32-C33-C34-C35
69	1B	205	3PE	C35-C36-C37-C38
69	1Y	201	3PE	C32-C33-C34-C35
69	3G	101	3PE	C39-C3A-C3B-C3C
75	1d	205	CDL	C34-C35-C36-C37
69	1A	201	3PE	C2D-C2E-C2F-C2G
69	1Y	209	3PE	C21-C22-C23-C24
88	4A	602	HEA	CAD-CBD-CGD-O2D
75	1q	202	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
75	3Y	106	CDL	C20-C21-C22-C23
75	4C	306	CDL	C62-C63-C64-C65
91	4J	101	PGV	O12-C04-C05-O05
82	1Y	203	PGT	C41-C42-C43-C44
69	1J	203	3PE	O32-C31-O31-C3
69	1l	204	3PE	C38-C39-C3A-C3B
69	1L	712	3PE	C39-C3A-C3B-C3C
75	1g	201	CDL	C75-C76-C77-C78
87	3X	102	PEK	C16-C17-C18-C19
69	3P	512	3PE	C22-C23-C24-C25
75	1Y	217	CDL	C41-C42-C43-C44
69	1g	202	3PE	C33-C34-C35-C36
69	1l	202	3PE	C23-C24-C25-C26
69	1m	205	3PE	C2-C1-O11-P
69	3G	104	3PE	C2-C1-O11-P
69	3G	105	3PE	C2-C1-O11-P
69	3J	104	3PE	C2-C1-O11-P
69	3R	305	3PE	C2-C1-O11-P
70	1A	202	PC1	C2-C1-O11-P
70	1Y	202	PC1	C2-C1-O11-P
70	1h	202	PC1	C2-C1-O11-P
75	3N	502	CDL	C1-CA2-OA2-PA1
69	1Y	213	3PE	C3A-C3B-C3C-C3D
70	1H	403	PC1	C2E-C2F-C2G-C2H
69	1m	201	3PE	C26-C27-C28-C29
69	3P	503	3PE	C2F-C2G-C2H-C2I
86	3Q	501	HEC	CAA-CBA-CGA-O2A
69	3X	106	3PE	C3C-C3D-C3E-C3F
69	3Q	502	3PE	C22-C21-O21-C2
69	1e	201	3PE	C39-C3A-C3B-C3C
69	3P	511	3PE	C34-C35-C36-C37
75	1g	201	CDL	C81-C82-C83-C84
88	4A	602	HEA	C2D-C3D-CAD-CBD
69	3P	515	3PE	C25-C26-C27-C28
69	3W	101	3PE	C3C-C3D-C3E-C3F
69	3P	511	3PE	C1-C2-C3-O31
69	3R	305	3PE	C1-C2-C3-O31
70	1B	203	PC1	C1-C2-C3-O31
75	4B	302	CDL	C17-C18-C19-C20
75	1d	205	CDL	C13-C14-C15-C16
91	4A	609	PGV	C12-C13-C14-C15
69	3C	515	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
69	1L	701	3PE	C28-C29-C2A-C2B
69	3X	108	3PE	C38-C39-C3A-C3B
70	1h	203	PC1	C35-C36-C37-C38
91	4G	102	PGV	C28-C29-C30-C31
69	1h	204	3PE	C27-C28-C29-C2A
75	1Y	217	CDL	C73-C74-C75-C76
69	1g	202	3PE	O11-C1-C2-O21
69	1m	201	3PE	O21-C21-C22-C23
69	3G	101	3PE	C34-C35-C36-C37
69	3G	102	3PE	C23-C24-C25-C26
70	1M	501	PC1	C2A-C2B-C2C-C2D
69	3Y	101	3PE	C36-C37-C38-C39
75	1g	201	CDL	C52-C53-C54-C55
87	4G	103	PEK	C14-C15-C16-C17
69	3C	511	3PE	C24-C25-C26-C27
91	4G	102	PGV	C30-C31-C32-C33
88	4A	602	HEA	CAD-CBD-CGD-O1D
75	1q	202	CDL	CB2-C1-CA2-OA2
69	1A	203	3PE	C22-C23-C24-C25
75	1N	402	CDL	C35-C36-C37-C38
75	3F	201	CDL	C77-C78-C79-C80
69	1d	201	3PE	C26-C27-C28-C29
69	1k	101	3PE	C33-C34-C35-C36
75	1g	201	CDL	C42-C43-C44-C45
91	4A	607	PGV	C27-C28-C29-C30
69	1Y	215	3PE	O11-C1-C2-C3
69	1l	203	3PE	O11-C1-C2-C3
69	3N	503	3PE	O11-C1-C2-C3
69	3R	305	3PE	O11-C1-C2-C3
70	1H	403	PC1	O11-C1-C2-C3
75	1L	704	CDL	OB5-CB3-CB4-CB6
75	1q	202	CDL	OA5-CA3-CA4-CA6
88	4A	602	HEA	C26-C15-C16-C17
69	3P	516	3PE	C32-C33-C34-C35
86	3D	501	HEC	C4D-C3D-CAD-CBD
69	3E	303	3PE	C21-C22-C23-C24
86	3D	501	HEC	CAA-CBA-CGA-O2A
75	1Y	217	CDL	C51-CB5-OB6-CB4
69	1B	204	3PE	C2F-C2G-C2H-C2I
69	1J	201	3PE	C2-C1-O11-P
69	1m	203	3PE	C2-C1-O11-P
69	1f	101	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
69	3P	505	3PE	C22-C23-C24-C25
82	1Y	203	PGT	C35-C36-C37-C38
69	1Y	213	3PE	C2D-C2E-C2F-C2G
69	4G	101	3PE	C24-C25-C26-C27
69	1Y	210	3PE	C24-C25-C26-C27
69	1g	202	3PE	C36-C37-C38-C39
69	1g	202	3PE	C2C-C2D-C2E-C2F
69	3Q	503	3PE	C29-C2A-C2B-C2C
69	3Q	504	3PE	C37-C38-C39-C3A
69	1Y	214	3PE	C2F-C2G-C2H-C2I
91	4C	303	PGV	C15-C16-C17-C18
69	1L	707	3PE	C27-C28-C29-C2A
69	1L	708	3PE	C36-C37-C38-C39
69	1m	202	3PE	C21-C22-C23-C24
69	3G	107	3PE	C21-C22-C23-C24
69	1Y	208	3PE	C3C-C3D-C3E-C3F
69	3R	304	3PE	C2F-C2G-C2H-C2I
69	1l	202	3PE	C24-C25-C26-C27
69	3C	508	3PE	C27-C28-C29-C2A
75	4C	307	CDL	C36-C37-C38-C39
69	1f	101	3PE	C3A-C3B-C3C-C3D
91	4C	305	PGV	C9-C10-C11-C12
70	1B	203	PC1	C27-C28-C29-C2A
70	1B	202	PC1	C35-C36-C37-C38
69	1f	104	3PE	C3B-C3C-C3D-C3E
70	1B	202	PC1	C36-C37-C38-C39
75	3X	103	CDL	C39-C40-C41-C42
69	3T	103	3PE	O32-C31-O31-C3
69	3P	518	3PE	C2D-C2E-C2F-C2G
70	1B	203	PC1	C32-C33-C34-C35
75	3F	201	CDL	C55-C56-C57-C58
75	4C	306	CDL	C15-C16-C17-C18
69	1e	201	3PE	C2C-C2D-C2E-C2F
69	3X	101	3PE	C35-C36-C37-C38
69	1J	201	3PE	O31-C31-C32-C33
69	3C	503	3PE	C34-C35-C36-C37
75	1Y	217	CDL	C75-C76-C77-C78
69	1L	706	3PE	C1-C2-O21-C21
69	1L	708	3PE	C1-C2-O21-C21
69	1l	202	3PE	C1-C2-O21-C21
69	3D	502	3PE	C3-C2-O21-C21
69	3Q	504	3PE	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
75	3X	103	CDL	CB3-CB4-OB6-CB5
69	1f	102	3PE	C2A-C2B-C2C-C2D
70	1H	403	PC1	C29-C2A-C2B-C2C
75	3X	103	CDL	C51-C52-C53-C54
75	4C	306	CDL	C23-C24-C25-C26
69	1L	709	3PE	C34-C35-C36-C37
69	1m	203	3PE	C28-C29-C2A-C2B
75	1L	704	CDL	C83-C84-C85-C86
69	1f	103	3PE	C25-C26-C27-C28
86	3Q	501	HEC	CAA-CBA-CGA-O1A
75	3X	103	CDL	C16-C17-C18-C19
75	4C	306	CDL	C34-C35-C36-C37
69	1J	203	3PE	C24-C25-C26-C27
69	3P	510	3PE	C3A-C3B-C3C-C3D
69	1L	701	3PE	C23-C24-C25-C26
75	3F	201	CDL	C11-C12-C13-C14
87	3X	102	PEK	C14-C15-C16-C17
91	4C	301	PGV	C11-C12-C13-C14
93	4B	303	PSC	C7-C8-C9-C10
83	1h	201	AME	CB-CA-N-CT1
69	3E	302	3PE	C25-C26-C27-C28
69	3Y	107	3PE	C2-C1-O11-P
75	1N	402	CDL	CB4-CB3-OB5-PB2
91	4N	101	PGV	C22-C23-C24-C25
69	1d	206	3PE	O21-C21-C22-C23
69	1J	201	3PE	C25-C26-C27-C28
69	3P	506	3PE	C24-C25-C26-C27
75	4B	302	CDL	C12-C13-C14-C15
69	3T	103	3PE	C32-C31-O31-C3
69	3C	507	3PE	C1-C2-C3-O31
69	3P	508	3PE	C1-C2-C3-O31
69	3X	108	3PE	C1-C2-C3-O31
75	1H	401	CDL	CA3-CA4-CA6-OA8
75	1d	205	CDL	CA3-CA4-CA6-OA8
69	3C	512	3PE	C23-C24-C25-C26
69	3W	101	3PE	C35-C36-C37-C38
69	1b	101	3PE	C22-C23-C24-C25
69	3P	518	3PE	C32-C33-C34-C35
69	3X	105	3PE	C3D-C3E-C3F-C3G
70	3T	102	PC1	C32-C31-O31-C3
87	3X	102	PEK	C3-C4-C5-C6
69	1A	203	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
91	4C	302	PGV	C24-C25-C26-C27
75	1N	402	CDL	OA7-CA5-OA6-CA4
69	3X	105	3PE	O31-C31-C32-C33
69	1d	206	3PE	C12-C11-O13-P
69	3P	518	3PE	C12-C11-O13-P
70	1P	502	PC1	C12-C11-O13-P
69	3Y	104	3PE	C3F-C3G-C3H-C3I
69	3C	512	3PE	C28-C29-C2A-C2B
69	3J	104	3PE	C36-C37-C38-C39
69	1N	401	3PE	C3F-C3G-C3H-C3I
69	3P	508	3PE	C2D-C2E-C2F-C2G
69	3P	517	3PE	C3B-C3C-C3D-C3E
69	3Y	101	3PE	C2A-C2B-C2C-C2D
75	1g	201	CDL	C61-C62-C63-C64
86	3D	501	HEC	CAA-CBA-CGA-O1A
69	3Q	503	3PE	C3A-C3B-C3C-C3D
69	3D	503	3PE	O31-C31-C32-C33
70	1H	402	PC1	O31-C31-C32-C33
75	1g	201	CDL	C32-C31-CA7-OA8
70	1M	501	PC1	C2D-C2E-C2F-C2G
91	4G	102	PGV	C25-C26-C27-C28
69	1L	702	3PE	O21-C2-C3-O31
69	1g	203	3PE	O21-C2-C3-O31
69	3P	508	3PE	O21-C2-C3-O31
75	3A	501	CDL	OA6-CA4-CA6-OA8
69	1N	401	3PE	C32-C33-C34-C35
91	4C	305	PGV	C23-C24-C25-C26
69	1Y	215	3PE	C2C-C2D-C2E-C2F
87	4G	103	PEK	C3-C4-C5-C6
91	4N	101	PGV	C9-C10-C11-C12
70	1h	202	PC1	O21-C21-C22-C23
75	1d	202	CDL	C32-C31-CA7-OA8
69	3A	502	3PE	C27-C28-C29-C2A
69	3G	107	3PE	C22-C23-C24-C25
69	3P	507	3PE	C39-C3A-C3B-C3C
69	1g	202	3PE	O11-C1-C2-C3
75	1Y	217	CDL	OB5-CB3-CB4-CB6
75	1d	205	CDL	OB5-CB3-CB4-CB6
75	3A	501	CDL	OB5-CB3-CB4-CB6
69	1J	201	3PE	C3E-C3F-C3G-C3H
82	1Y	203	PGT	C43-C44-C45-C46
69	3Y	104	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
70	1Y	207	PC1	C2B-C2C-C2D-C2E
69	3P	505	3PE	C32-C33-C34-C35
91	4A	609	PGV	C20-C21-C22-C23
70	1M	501	PC1	O21-C21-C22-C23
75	1q	201	CDL	C52-C51-CB5-OB6
91	4J	101	PGV	C19-C20-C21-C22
69	3T	103	3PE	C3A-C3B-C3C-C3D
69	3P	507	3PE	C32-C33-C34-C35
69	1N	401	3PE	C28-C29-C2A-C2B
69	3P	512	3PE	C3A-C3B-C3C-C3D
75	1d	202	CDL	C54-C55-C56-C57
69	1L	712	3PE	C28-C29-C2A-C2B
69	3R	304	3PE	C3C-C3D-C3E-C3F
69	3W	103	3PE	C22-C23-C24-C25
70	1H	403	PC1	C21-C22-C23-C24
70	1h	203	PC1	C22-C23-C24-C25
69	1f	101	3PE	O21-C21-C22-C23
69	1h	204	3PE	O21-C21-C22-C23
69	3C	508	3PE	O31-C31-C32-C33
69	3T	103	3PE	C2E-C2F-C2G-C2H
69	3X	101	3PE	C33-C34-C35-C36
69	3Y	101	3PE	C35-C36-C37-C38
69	1L	703	3PE	O32-C31-O31-C3
69	3P	503	3PE	C3D-C3E-C3F-C3G
69	3C	505	3PE	C2-C1-O11-P
69	3T	103	3PE	C2-C1-O11-P
75	1q	202	CDL	CB4-CB3-OB5-PB2
70	1h	202	PC1	C25-C26-C27-C28
75	1g	201	CDL	C79-C80-C81-C82
69	3A	502	3PE	C2A-C2B-C2C-C2D
69	3E	303	3PE	C2E-C2F-C2G-C2H
91	4C	302	PGV	C20-C21-C22-C23
91	4C	302	PGV	C26-C27-C28-C29
69	3C	508	3PE	O21-C21-C22-C23
75	1N	402	CDL	C32-C31-CA7-OA8
75	3N	502	CDL	C12-C11-CA5-OA6
91	4J	101	PGV	O03-C19-C20-C21
69	3W	103	3PE	C28-C29-C2A-C2B
69	3P	514	3PE	C3C-C3D-C3E-C3F
77	1O	401	GTP	PA-O3A-PB-O2B
69	3C	511	3PE	C31-C32-C33-C34
75	1q	202	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
70	3X	104	PC1	C32-C33-C34-C35
81	1n	201	EHZ	C7-C8-C9-O2
69	3N	501	3PE	C3C-C3D-C3E-C3F
75	1N	402	CDL	C11-CA5-OA6-CA4
75	1q	202	CDL	C11-CA5-OA6-CA4
69	1b	101	3PE	C25-C26-C27-C28
70	3T	102	PC1	O32-C31-O31-C3
69	3P	503	3PE	O21-C21-C22-C23
75	1Y	217	CDL	C54-C55-C56-C57
75	1d	202	CDL	C16-C17-C18-C19
75	1Y	217	CDL	C24-C25-C26-C27
69	3P	514	3PE	C2E-C2F-C2G-C2H
69	3R	302	3PE	C37-C38-C39-C3A
69	3C	512	3PE	C3C-C3D-C3E-C3F
69	3C	507	3PE	O31-C31-C32-C33
69	3R	304	3PE	C33-C34-C35-C36
70	1d	204	PC1	O11-C1-C2-O21
75	1d	202	CDL	OB5-CB3-CB4-OB6
75	3X	103	CDL	OA5-CA3-CA4-OA6
75	4C	307	CDL	OA5-CA3-CA4-OA6
81	1n	201	EHZ	O4-C15-C16-C17
69	3Y	101	3PE	C25-C26-C27-C28
70	1Y	202	PC1	C21-C22-C23-C24
75	3T	101	CDL	C73-C74-C75-C76
69	3J	105	3PE	O21-C21-C22-C23
69	3J	105	3PE	C3A-C3B-C3C-C3D
69	3P	506	3PE	C3B-C3C-C3D-C3E
85	3P	502	HEM	CAD-CBD-CGD-O1D
69	3W	101	3PE	C3E-C3F-C3G-C3H
70	3X	104	PC1	C21-C22-C23-C24
69	1L	707	3PE	C33-C34-C35-C36
69	1J	203	3PE	C27-C28-C29-C2A
69	3Y	104	3PE	C24-C25-C26-C27
75	1q	202	CDL	C75-C76-C77-C78
69	1m	201	3PE	C3F-C3G-C3H-C3I
75	4C	306	CDL	C72-C71-CB7-OB8
69	3Y	104	3PE	C3C-C3D-C3E-C3F
69	3Y	104	3PE	O32-C31-O31-C3
69	1L	702	3PE	C1-C2-C3-O31
69	3C	511	3PE	C1-C2-C3-O31
75	3F	201	CDL	CB3-CB4-CB6-OB8
88	4A	601	HEA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
69	1f	104	3PE	C23-C24-C25-C26
69	3G	107	3PE	C32-C33-C34-C35
70	1H	402	PC1	C11-C12-N-C14
69	3P	512	3PE	C28-C29-C2A-C2B
70	3X	104	PC1	C36-C37-C38-C39
75	1d	205	CDL	C79-C80-C81-C82
69	3G	101	3PE	C33-C34-C35-C36
70	1Y	207	PC1	C26-C27-C28-C29
69	3G	111	3PE	O21-C21-C22-C23
75	1d	205	CDL	C52-C51-CB5-OB6
75	3F	201	CDL	C72-C71-CB7-OB8
75	3F	201	CDL	OA6-CA4-CA6-OA8
75	3T	101	CDL	OA6-CA4-CA6-OA8
69	3D	503	3PE	C26-C27-C28-C29
69	3P	517	3PE	C3D-C3E-C3F-C3G
69	1B	205	3PE	C2D-C2E-C2F-C2G
69	1d	203	3PE	C25-C26-C27-C28
69	3P	515	3PE	C3D-C3E-C3F-C3G
75	1Y	217	CDL	C51-C52-C53-C54
75	1q	201	CDL	C31-CA7-OA8-CA6
69	1d	201	3PE	O31-C31-C32-C33
82	1Y	203	PGT	O2-C31-C32-C33
69	3P	510	3PE	C2A-C2B-C2C-C2D
70	1Y	206	PC1	C3B-C3C-C3D-C3E
75	1Y	217	CDL	C14-C15-C16-C17
69	1l	203	3PE	C31-C32-C33-C34
69	1B	205	3PE	C3C-C3D-C3E-C3F
75	1d	205	CDL	C83-C84-C85-C86
69	1m	202	3PE	C25-C26-C27-C28
70	3J	106	PC1	C34-C35-C36-C37
84	1l	201	MYR	C3-C4-C5-C6
69	3W	103	3PE	C23-C24-C25-C26
69	1Y	216	3PE	C35-C36-C37-C38
69	4G	104	3PE	C24-C25-C26-C27
75	1Y	217	CDL	C32-C33-C34-C35
75	4C	306	CDL	C63-C64-C65-C66
69	3C	514	3PE	C31-C32-C33-C34
69	1l	202	3PE	O21-C21-C22-C23
69	3Y	107	3PE	C38-C39-C3A-C3B
81	1T	101	EHZ	C1-C2-C3-C4
75	3X	103	CDL	CA2-C1-CB2-OB2
69	3A	503	3PE	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
69	3C	504	3PE	C2-C3-O31-C31
69	1L	702	3PE	O31-C31-C32-C33
75	4C	307	CDL	C23-C24-C25-C26
69	3Y	104	3PE	C32-C31-O31-C3
69	1Y	208	3PE	C26-C27-C28-C29
75	1d	202	CDL	C38-C39-C40-C41
75	4B	302	CDL	C43-C44-C45-C46
69	3Y	104	3PE	C31-C32-C33-C34
69	3E	303	3PE	C33-C34-C35-C36
75	3F	201	CDL	C31-C32-C33-C34
69	1L	710	3PE	C3-C2-O21-C21
69	3C	505	3PE	C1-C2-O21-C21
69	3D	502	3PE	C1-C2-O21-C21
69	1L	705	3PE	C34-C35-C36-C37
75	3Y	106	CDL	C31-C32-C33-C34
82	1Y	203	PGT	C32-C33-C34-C35
69	3G	110	3PE	C28-C29-C2A-C2B
69	3P	516	3PE	C3E-C3F-C3G-C3H
91	4G	102	PGV	O03-C19-C20-C21
75	1g	201	CDL	C34-C35-C36-C37
69	3G	105	3PE	C34-C35-C36-C37
69	3P	519	3PE	C27-C28-C29-C2A
69	3R	305	3PE	C36-C37-C38-C39
70	3R	303	PC1	C2B-C2C-C2D-C2E
70	1Y	202	PC1	C26-C27-C28-C29
70	1H	403	PC1	C24-C25-C26-C27
69	3C	515	3PE	C35-C36-C37-C38
75	1g	201	CDL	C32-C31-CA7-OA9
69	3Y	101	3PE	C29-C2A-C2B-C2C
75	3D	504	CDL	C72-C73-C74-C75
81	1T	101	EHZ	C2-C3-C4-C5
69	3Y	104	3PE	C21-C22-C23-C24
75	1d	205	CDL	C1-CA2-OA2-PA1
91	4C	302	PGV	C02-C03-O11-P
85	3P	502	HEM	CAD-CBD-CGD-O2D
75	3Y	106	CDL	C63-C64-C65-C66
75	1N	402	CDL	C32-C31-CA7-OA9
69	3P	520	3PE	C29-C2A-C2B-C2C
69	1Y	209	3PE	O31-C31-C32-C33
69	3P	511	3PE	C26-C27-C28-C29
69	1Y	205	3PE	C24-C25-C26-C27
69	3X	107	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
70	3P	509	PC1	C37-C38-C39-C3A
75	1q	202	CDL	C52-C53-C54-C55
69	3C	507	3PE	O32-C31-C32-C33
69	3P	503	3PE	O22-C21-C22-C23
69	3C	511	3PE	O11-C1-C2-O21
69	3G	109	3PE	C26-C27-C28-C29
69	3P	504	3PE	C35-C36-C37-C38
69	3P	508	3PE	C38-C39-C3A-C3B
75	3N	502	CDL	C78-C79-C80-C81
75	3T	101	CDL	C51-C52-C53-C54
75	3N	502	CDL	C81-C82-C83-C84
69	3G	110	3PE	C2C-C2D-C2E-C2F
91	4N	101	PGV	C11-C12-C13-C14
69	1Z	201	3PE	C23-C24-C25-C26
69	3P	518	3PE	C3E-C3F-C3G-C3H
70	3J	106	PC1	C28-C29-C2A-C2B
75	3A	501	CDL	C32-C33-C34-C35
69	1g	202	3PE	C2D-C2E-C2F-C2G
69	1l	204	3PE	C2E-C2F-C2G-C2H
69	3J	103	3PE	C32-C31-O31-C3
70	1P	502	PC1	C11-C12-N-C13
70	1d	204	PC1	O31-C31-C32-C33
69	3G	111	3PE	O22-C21-C22-C23
75	1d	202	CDL	C32-C31-CA7-OA9
69	3Q	503	3PE	C26-C27-C28-C29
69	3Q	504	3PE	C35-C36-C37-C38
75	1d	205	CDL	C74-C75-C76-C77
75	3A	501	CDL	C17-C18-C19-C20
91	4N	101	PGV	C13-C14-C15-C16
75	3F	201	CDL	C17-C18-C19-C20
75	1q	202	CDL	O1-C1-CA2-OA2
69	3P	503	3PE	C2D-C2E-C2F-C2G
69	1f	101	3PE	O22-C21-C22-C23
75	1q	201	CDL	C52-C51-CB5-OB7
69	3Y	107	3PE	C2E-C2F-C2G-C2H
69	1L	708	3PE	O32-C31-O31-C3
69	1h	204	3PE	O22-C21-C22-C23
69	1l	202	3PE	C34-C35-C36-C37
69	3P	507	3PE	C2F-C2G-C2H-C2I
69	3J	103	3PE	C3D-C3E-C3F-C3G
69	3C	506	3PE	C2F-C2G-C2H-C2I
70	1d	204	PC1	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
69	1L	709	3PE	C37-C38-C39-C3A
69	1L	710	3PE	C36-C37-C38-C39
69	3X	105	3PE	C26-C27-C28-C29
75	1q	202	CDL	C72-C73-C74-C75
69	3C	515	3PE	O21-C21-C22-C23
75	1q	202	CDL	C12-C11-CA5-OA6
75	3X	103	CDL	C72-C71-CB7-OB8
69	1Y	216	3PE	C3B-C3C-C3D-C3E
88	4A	602	HEA	C4D-C3D-CAD-CBD
69	3C	508	3PE	O32-C31-C32-C33
69	3X	105	3PE	O32-C31-C32-C33
70	1M	501	PC1	O22-C21-C22-C23
70	1h	202	PC1	O22-C21-C22-C23
91	4G	102	PGV	O04-C19-C20-C21
75	4B	302	CDL	C44-C45-C46-C47
75	3X	103	CDL	C53-C54-C55-C56
69	3C	517	3PE	O22-C21-O21-C2
69	3P	517	3PE	O21-C2-C3-O31
75	3F	201	CDL	OB6-CB4-CB6-OB8
75	3Y	106	CDL	C60-C61-C62-C63
70	1Y	202	PC1	C25-C26-C27-C28
75	3Y	106	CDL	C14-C15-C16-C17
69	1L	702	3PE	O32-C31-C32-C33
75	3N	502	CDL	C12-C11-CA5-OA7
91	4J	101	PGV	O04-C19-C20-C21
69	3G	104	3PE	O21-C21-C22-C23
70	1B	203	PC1	O21-C21-C22-C23
75	3F	201	CDL	C80-C81-C82-C83
75	1q	201	CDL	OA9-CA7-OA8-CA6
69	3C	503	3PE	C28-C29-C2A-C2B
69	3X	107	3PE	C22-C23-C24-C25
82	1Y	203	PGT	C40-C41-C42-C43
69	3D	503	3PE	O32-C31-C32-C33
70	1H	402	PC1	O32-C31-C32-C33
70	1M	501	PC1	C2-C1-O11-P
75	4B	302	CDL	C1-CB2-OB2-PB2
69	3X	105	3PE	O21-C21-C22-C23
70	1H	402	PC1	C11-C12-N-C13
70	1H	402	PC1	C11-C12-N-C15
69	1J	201	3PE	C33-C34-C35-C36
91	4C	303	PGV	C30-C31-C32-C33
69	3C	508	3PE	O22-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	3J	105	3PE	O22-C21-C22-C23
69	1L	702	3PE	C29-C2A-C2B-C2C
69	3G	101	3PE	C2E-C2F-C2G-C2H
75	4C	307	CDL	C77-C78-C79-C80
69	3C	516	3PE	C23-C24-C25-C26
69	3T	103	3PE	C2C-C2D-C2E-C2F
75	1d	205	CDL	O1-C1-CB2-OB2
91	4N	101	PGV	C29-C30-C31-C32
75	1d	202	CDL	OA9-CA7-OA8-CA6
69	3P	508	3PE	C35-C36-C37-C38
75	3P	513	CDL	C79-C80-C81-C82
91	4N	101	PGV	C2-C3-C4-C5
69	3G	111	3PE	O11-C1-C2-C3
69	3W	103	3PE	O11-C1-C2-C3
82	1Y	203	PGT	O31-C31-C32-C33
69	3J	104	3PE	O21-C21-C22-C23
75	3Y	106	CDL	C52-C51-CB5-OB6
69	3C	503	3PE	C2B-C2C-C2D-C2E
69	1L	712	3PE	C37-C38-C39-C3A
69	1f	102	3PE	C2C-C2D-C2E-C2F
70	1d	204	PC1	O32-C31-C32-C33
75	1d	205	CDL	C52-C51-CB5-OB7
69	3D	503	3PE	C21-C22-C23-C24
70	3P	509	PC1	C31-C32-C33-C34
69	3C	512	3PE	C26-C27-C28-C29
69	3Y	101	3PE	C23-C24-C25-C26
69	1Y	205	3PE	O21-C21-C22-C23
69	1Y	211	3PE	O31-C31-C32-C33
69	3C	507	3PE	O21-C21-C22-C23
70	1A	202	PC1	O31-C31-C32-C33
76	1I	203	AYA	CB-CA-N-CT
75	3X	103	CDL	C60-C61-C62-C63
69	1l	202	3PE	O22-C21-C22-C23
70	1B	203	PC1	O22-C21-C22-C23
69	1Z	201	3PE	C25-C26-C27-C28
69	4G	101	3PE	C23-C24-C25-C26
69	3P	511	3PE	C39-C3A-C3B-C3C
69	1f	102	3PE	C33-C34-C35-C36
69	1l	204	3PE	C2B-C2C-C2D-C2E
69	1L	710	3PE	O31-C31-C32-C33
69	3C	506	3PE	O21-C21-C22-C23
69	3P	517	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
69	4G	101	3PE	O21-C21-C22-C23
69	1L	703	3PE	C32-C31-O31-C3
69	3S	201	3PE	C2A-C2B-C2C-C2D
69	3C	513	3PE	C3F-C3G-C3H-C3I
69	1f	102	3PE	C21-C22-C23-C24
69	1f	104	3PE	C21-C22-C23-C24
75	1q	202	CDL	C12-C11-CA5-OA7
75	4C	306	CDL	C57-C58-C59-C60

There are no ring outliers.

214 monomers are involved in 3448 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	3P	507	3PE	21	0
69	3R	304	3PE	18	0
69	3E	303	3PE	13	0
70	1Y	207	PC1	34	0
75	3X	103	CDL	31	0
69	1L	708	3PE	10	0
69	3G	107	3PE	10	0
69	3X	107	3PE	26	0
69	3C	511	3PE	35	0
75	1H	401	CDL	10	0
75	3T	101	CDL	13	0
81	1n	201	EHZ	1	0
91	4C	303	PGV	19	0
69	3W	102	3PE	25	0
69	3N	501	3PE	38	0
72	1E	301	FES	4	0
69	3C	506	3PE	17	0
69	3J	102	3PE	1	0
69	3P	508	3PE	23	0
69	3N	503	3PE	28	0
69	3P	510	3PE	20	0
75	4C	306	CDL	19	0
69	1A	203	3PE	20	0
69	1Y	211	3PE	19	0
91	4K	101	PGV	7	0
69	3G	103	3PE	14	0
69	1Y	208	3PE	57	0
69	3Q	502	3PE	11	0
71	1I	201	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	3E	302	3PE	14	0
70	1Y	206	PC1	39	0
69	3X	106	3PE	9	0
69	1Y	214	3PE	35	0
69	1Y	216	3PE	14	0
83	1h	201	AME	2	0
93	4B	303	PSC	27	0
91	4A	607	PGV	11	0
69	3X	101	3PE	26	0
85	3C	502	HEM	4	0
69	3C	507	3PE	23	0
69	1L	712	3PE	17	0
69	1l	203	3PE	11	0
69	3C	510	3PE	9	0
69	3X	108	3PE	39	0
79	1P	501	NDP	2	0
69	3P	517	3PE	21	0
69	1Y	205	3PE	17	0
69	1Y	201	3PE	23	0
69	3S	201	3PE	26	0
85	3P	502	HEM	4	0
69	3Q	503	3PE	18	0
76	1I	203	AYA	6	0
69	3C	503	3PE	10	0
69	1L	705	3PE	15	0
75	3F	201	CDL	26	0
86	3D	501	HEC	6	0
69	3P	516	3PE	11	0
69	3G	102	3PE	9	0
69	3R	302	3PE	18	0
69	1N	401	3PE	57	0
69	3C	514	3PE	4	0
69	1l	204	3PE	12	0
69	3P	512	3PE	17	0
69	1L	706	3PE	17	0
70	1P	502	PC1	6	0
69	3G	110	3PE	18	0
69	1d	203	3PE	24	0
69	1m	202	3PE	23	0
88	4A	601	HEA	7	0
69	3G	109	3PE	21	0
69	1m	201	3PE	13	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	3P	504	3PE	12	0
69	1f	102	3PE	19	0
88	4A	602	HEA	4	0
70	1H	404	PC1	19	0
69	1Y	215	3PE	31	0
69	3Y	104	3PE	11	0
69	1d	206	3PE	32	0
91	4A	606	PGV	14	0
75	1q	201	CDL	11	0
69	3P	506	3PE	14	0
72	3E	301	FES	5	0
69	1L	703	3PE	29	0
69	1L	710	3PE	18	0
75	1d	205	CDL	28	0
69	1l	202	3PE	6	0
69	1g	203	3PE	13	0
87	4G	103	PEK	13	0
69	3P	519	3PE	24	0
69	1d	201	3PE	48	0
69	1f	104	3PE	77	0
70	3R	303	PC1	16	0
70	1B	202	PC1	66	0
70	3T	102	PC1	45	0
69	1o	201	3PE	31	0
69	1Y	212	3PE	20	0
70	1B	203	PC1	22	0
75	4B	302	CDL	40	0
72	1G	803	FES	4	0
71	1B	201	SF4	1	0
85	3C	501	HEM	4	0
87	3X	102	PEK	9	0
91	4N	101	PGV	13	0
91	4A	609	PGV	60	0
69	3A	503	3PE	27	0
69	3C	515	3PE	24	0
75	1q	202	CDL	29	0
69	1e	201	3PE	15	0
75	1L	704	CDL	38	0
69	3P	505	3PE	9	0
70	1d	204	PC1	24	0
73	1F	501	FMN	4	0
69	3G	108	3PE	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
75	4C	307	CDL	22	0
69	3R	305	3PE	23	0
69	3P	503	3PE	27	0
69	3P	518	3PE	24	0
69	3G	101	3PE	12	0
69	3P	515	3PE	11	0
70	1M	501	PC1	12	0
69	1b	101	3PE	31	0
69	3C	508	3PE	22	0
69	3G	105	3PE	13	0
69	1B	204	3PE	25	0
91	4G	102	PGV	10	0
69	3G	104	3PE	12	0
69	1B	205	3PE	26	0
69	1L	707	3PE	10	0
69	1m	204	3PE	5	0
69	1Y	210	3PE	9	0
69	3C	512	3PE	57	0
69	3G	111	3PE	8	0
71	1G	802	SF4	4	0
86	3Q	501	HEC	10	0
69	1k	101	3PE	32	0
69	3P	514	3PE	43	0
69	3C	517	3PE	16	0
69	3C	509	3PE	22	0
69	1f	101	3PE	14	0
69	3C	504	3PE	5	0
71	1F	502	SF4	8	0
69	1L	701	3PE	14	0
69	1L	702	3PE	9	0
69	4G	101	3PE	12	0
72	3R	301	FES	4	0
69	1J	203	3PE	17	0
75	3N	502	CDL	57	0
69	3Y	103	3PE	9	0
69	3Y	105	3PE	40	0
70	1h	203	PC1	13	0
69	1L	709	3PE	24	0
69	3J	104	3PE	20	0
91	4C	302	PGV	19	0
75	3D	504	CDL	4	0
91	4C	305	PGV	14	0

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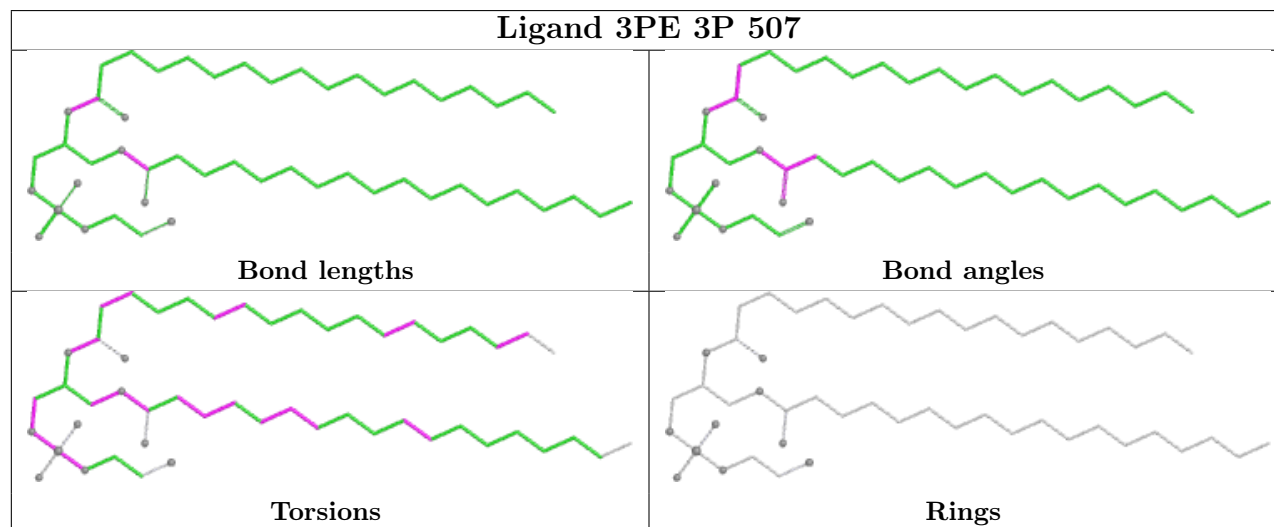
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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69	3D	503	3PE	13	0
69	1Y	209	3PE	25	0
69	1m	205	3PE	24	0
82	1Y	203	PGT	24	0
69	3J	103	3PE	20	0
69	3J	105	3PE	16	0
69	1L	711	3PE	14	0
69	3P	511	3PE	27	0
69	3A	502	3PE	34	0
75	1d	202	CDL	32	0
69	1Y	204	3PE	11	0
69	3T	103	3PE	26	0
69	3G	106	3PE	6	0
70	3J	106	PC1	13	0
70	1H	402	PC1	18	0
70	1A	202	PC1	28	0
70	1h	202	PC1	16	0
91	4C	301	PGV	5	0
69	3Y	107	3PE	28	0
69	3P	520	3PE	26	0
75	1g	201	CDL	60	0
70	3P	509	PC1	15	0
69	1h	204	3PE	15	0
69	3C	513	3PE	41	0
69	3Y	102	3PE	21	0
70	1J	202	PC1	7	0
69	3Q	504	3PE	14	0
75	3P	513	CDL	60	0
77	1O	401	GTP	7	0
75	3A	501	CDL	45	0
69	3J	101	3PE	11	0
91	4A	608	PGV	19	0
85	3P	501	HEM	1	0
70	1H	403	PC1	21	0
69	3W	101	3PE	23	0
69	3D	502	3PE	6	0
91	4J	101	PGV	8	0
69	1Z	201	3PE	12	0
69	1f	103	3PE	16	0
69	1g	202	3PE	30	0
70	1Y	202	PC1	11	0

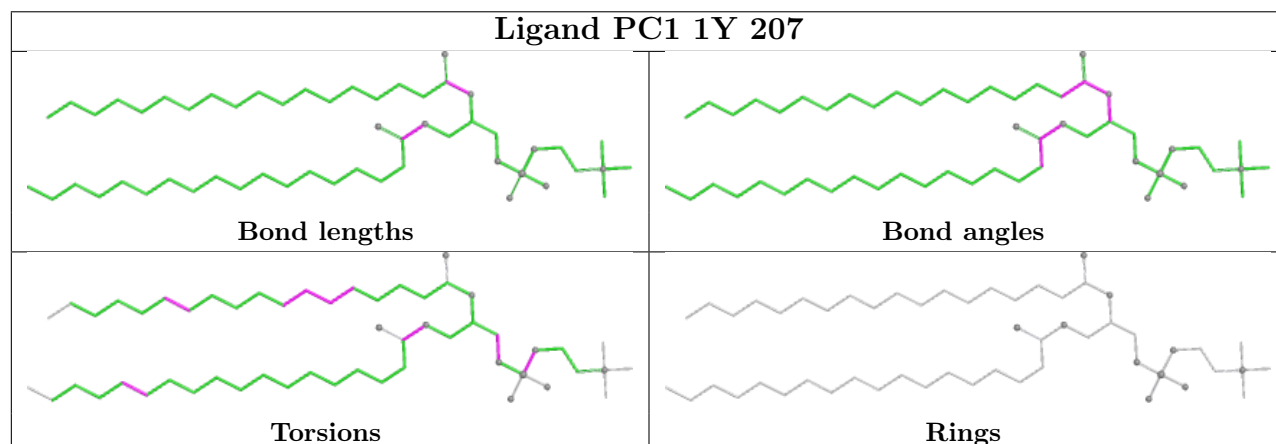
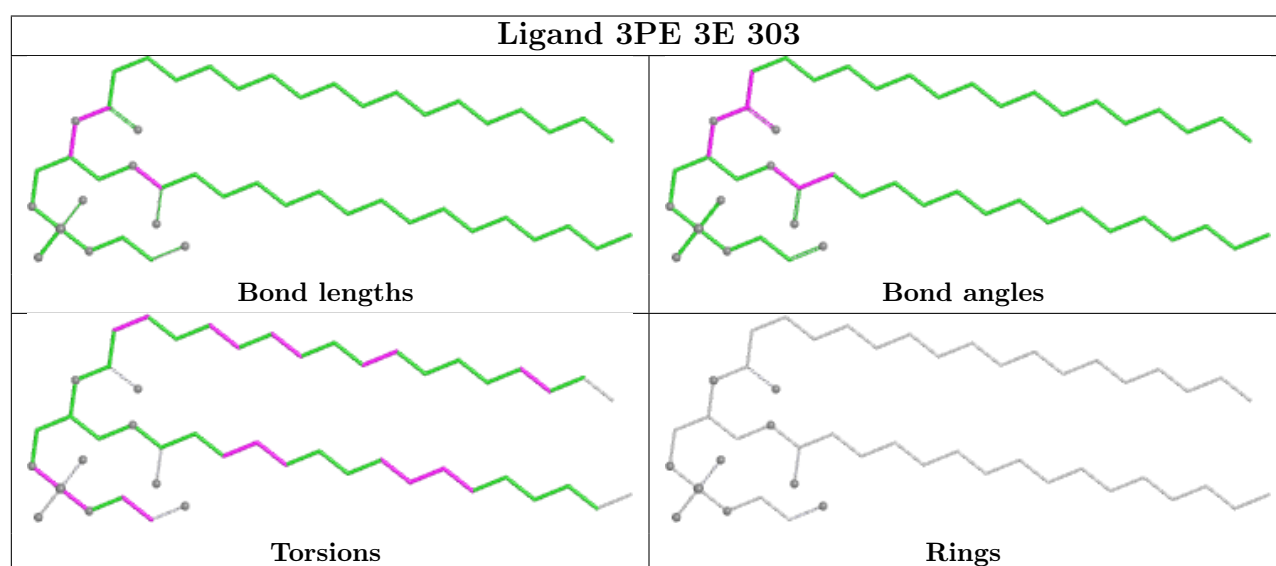
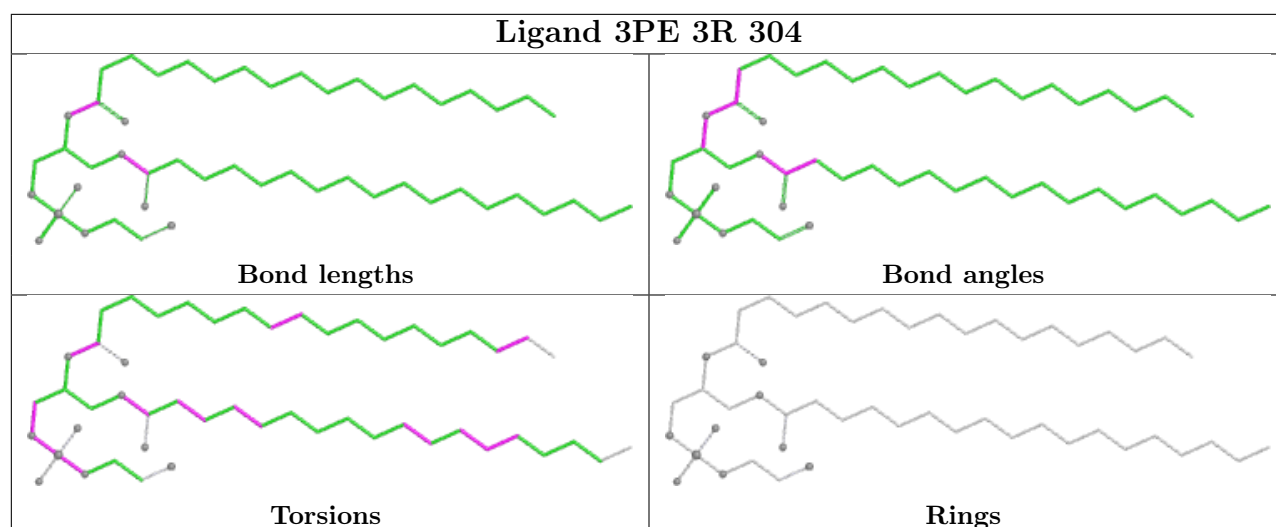
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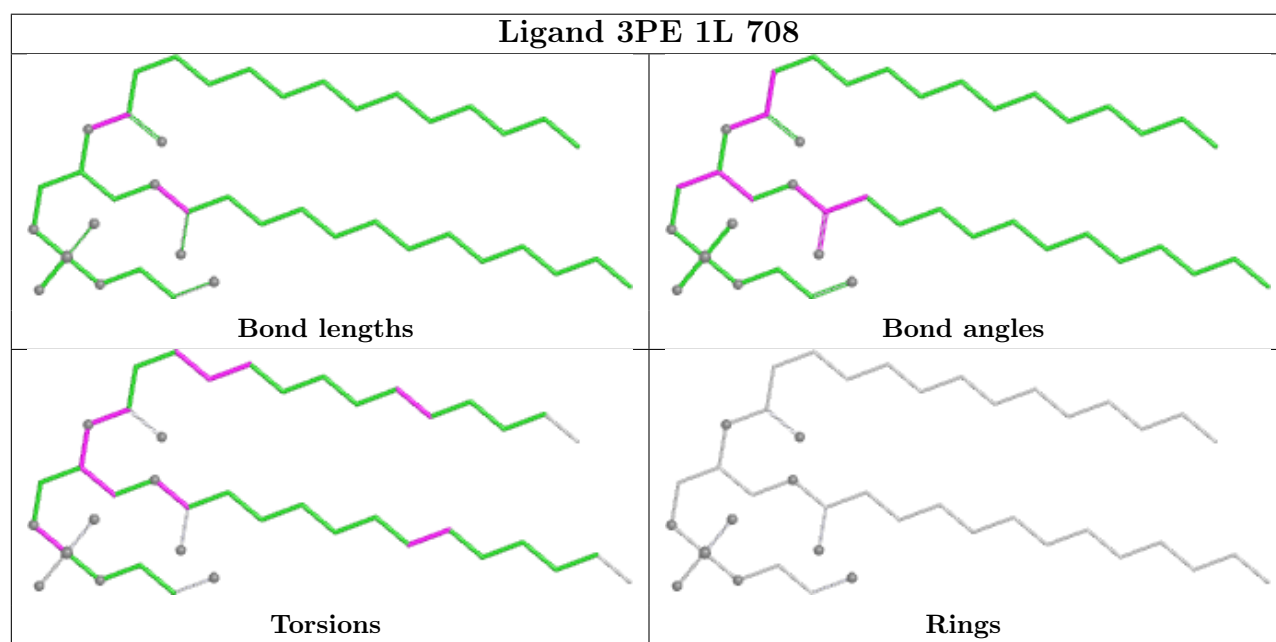
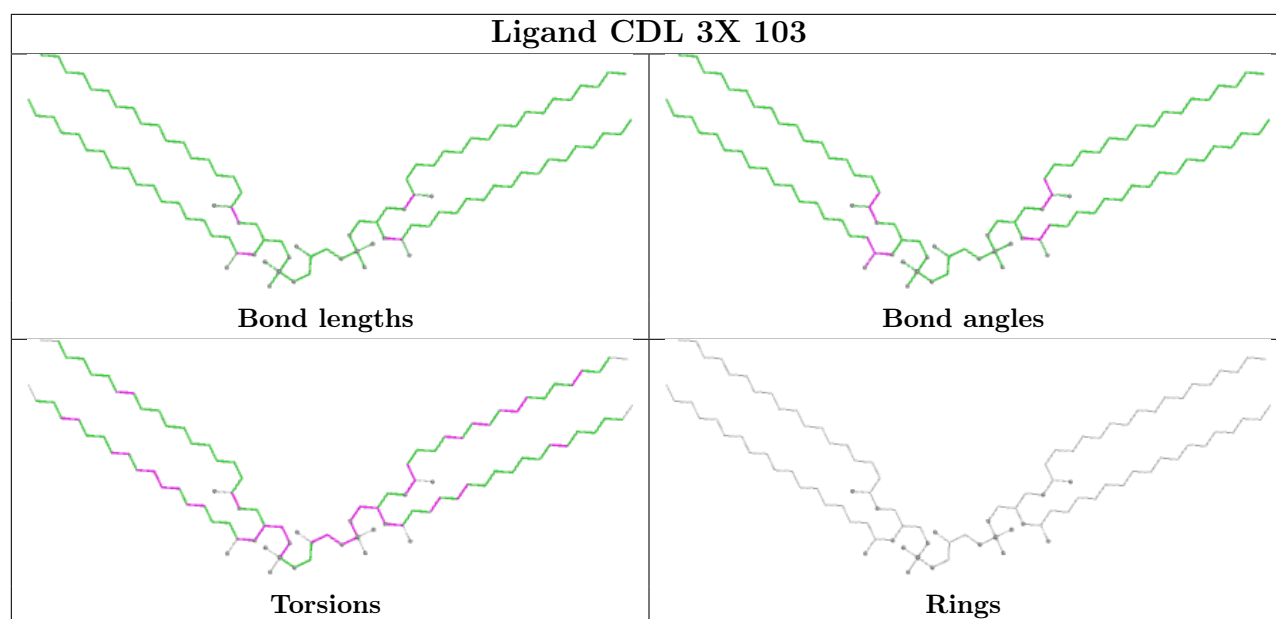
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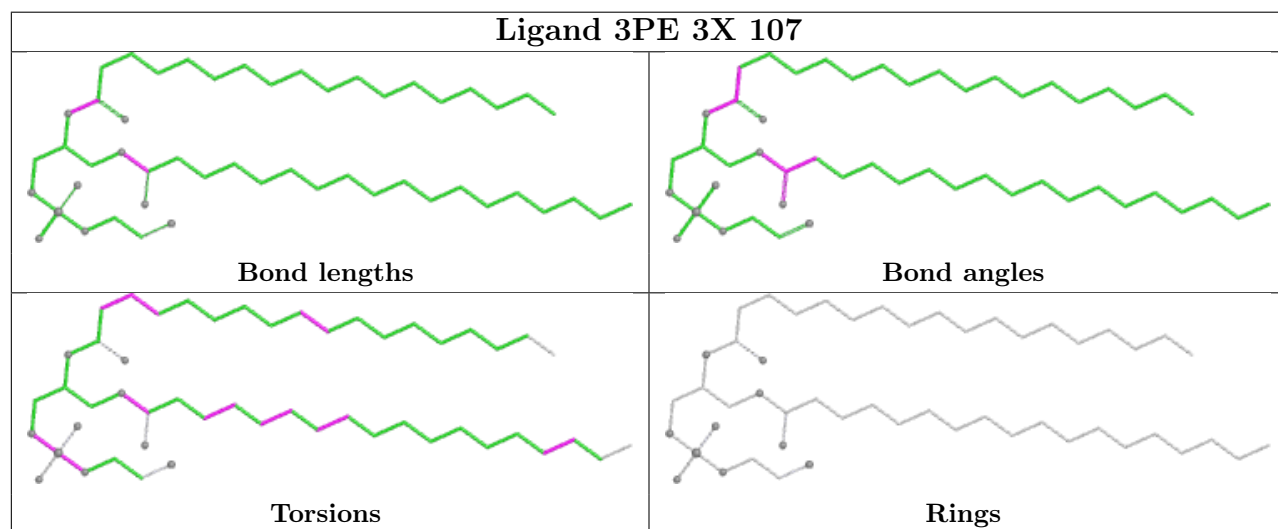
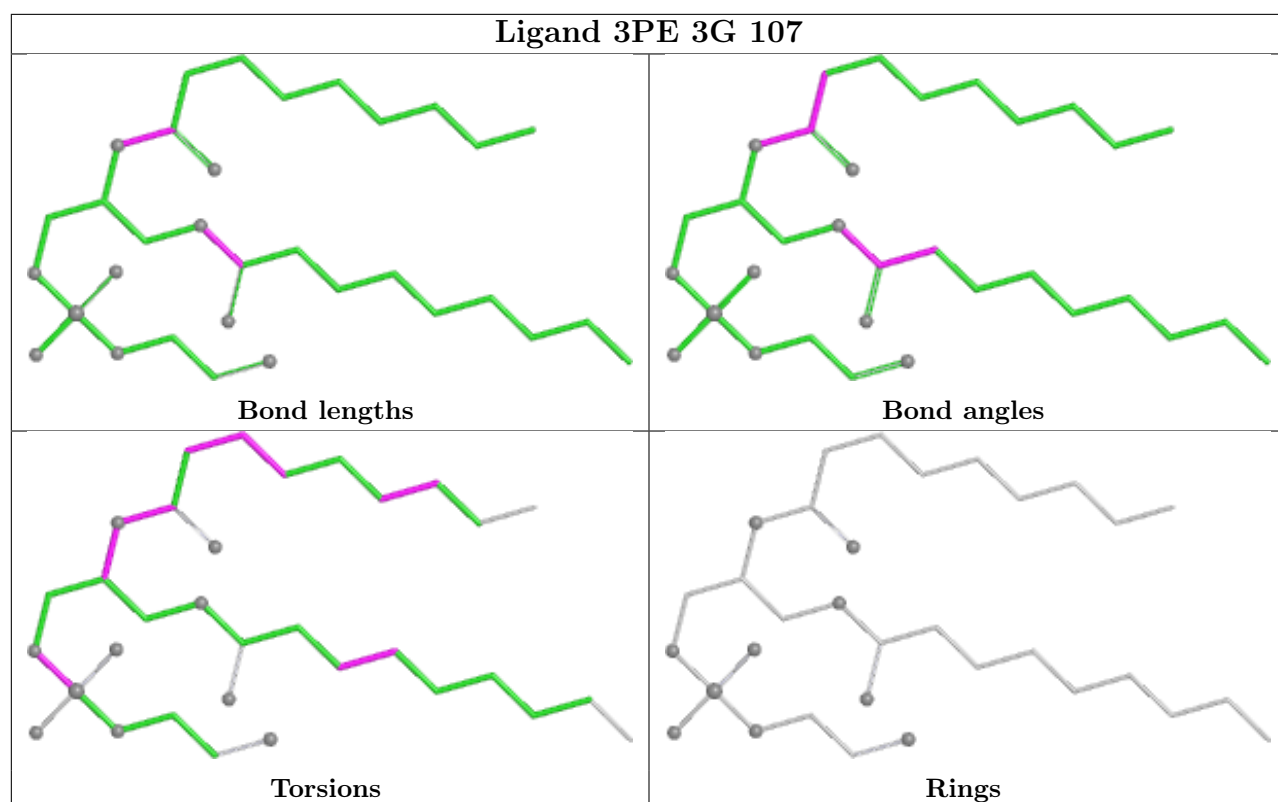
Mol	Chain	Res	Type	Clashes	Symm-Clashes
69	4G	104	3PE	25	0
69	3W	103	3PE	27	0
91	4C	304	PGV	9	0
69	1Y	213	3PE	21	0
71	1I	202	SF4	2	0
69	3Y	101	3PE	15	0
75	1Y	217	CDL	39	0
69	3X	105	3PE	24	0
75	3Y	106	CDL	31	0
69	1A	201	3PE	13	0
69	1m	203	3PE	34	0
69	3C	505	3PE	6	0
75	1N	402	CDL	33	0
75	1i	201	CDL	35	0
69	1J	201	3PE	37	0
70	3X	104	PC1	17	0
69	3C	516	3PE	24	0

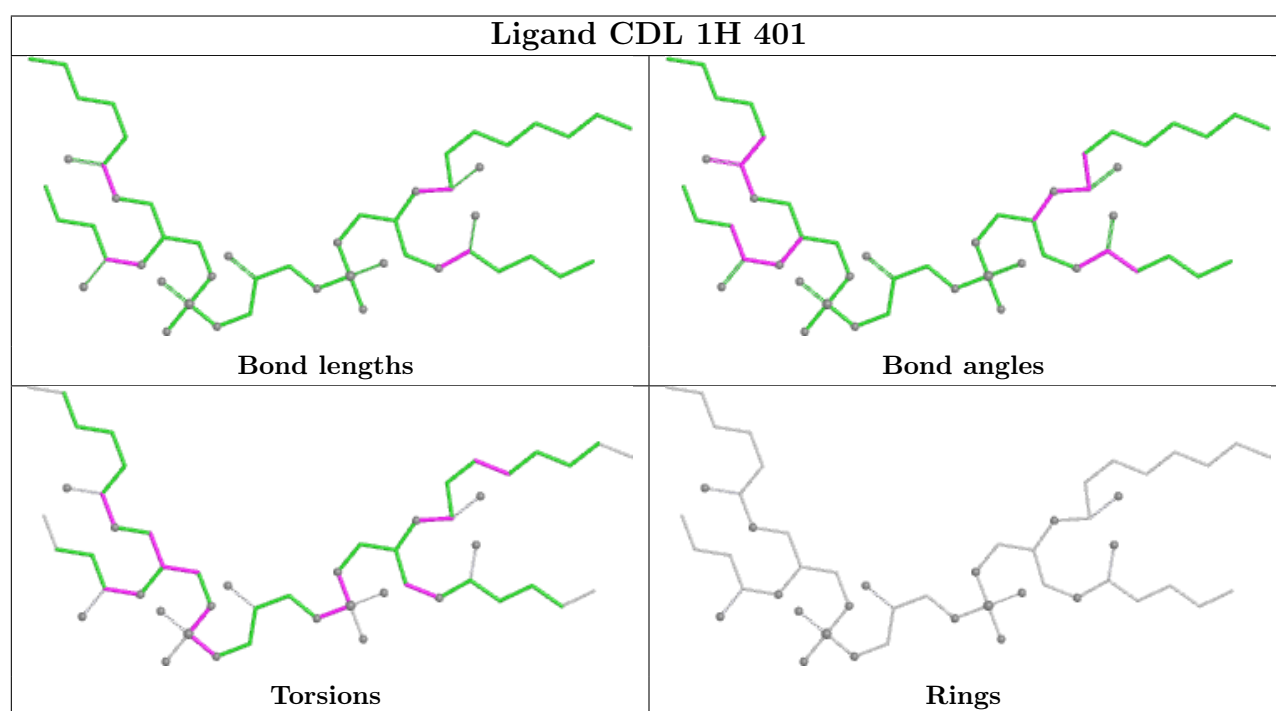
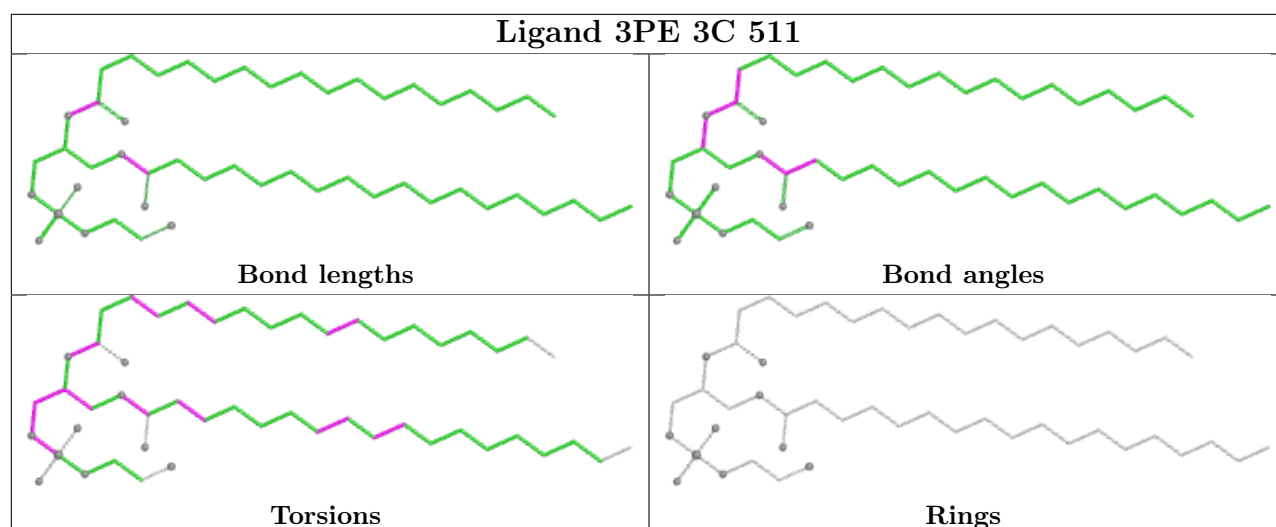
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

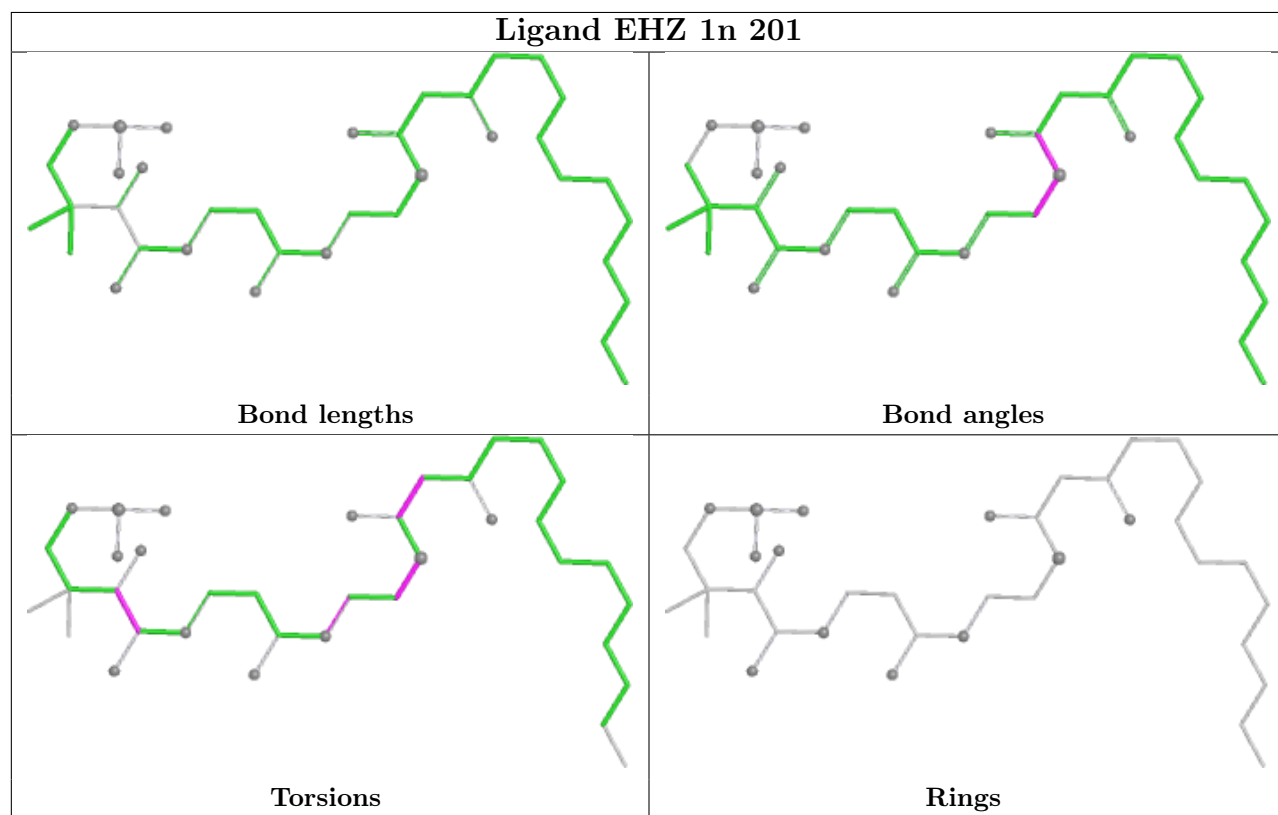
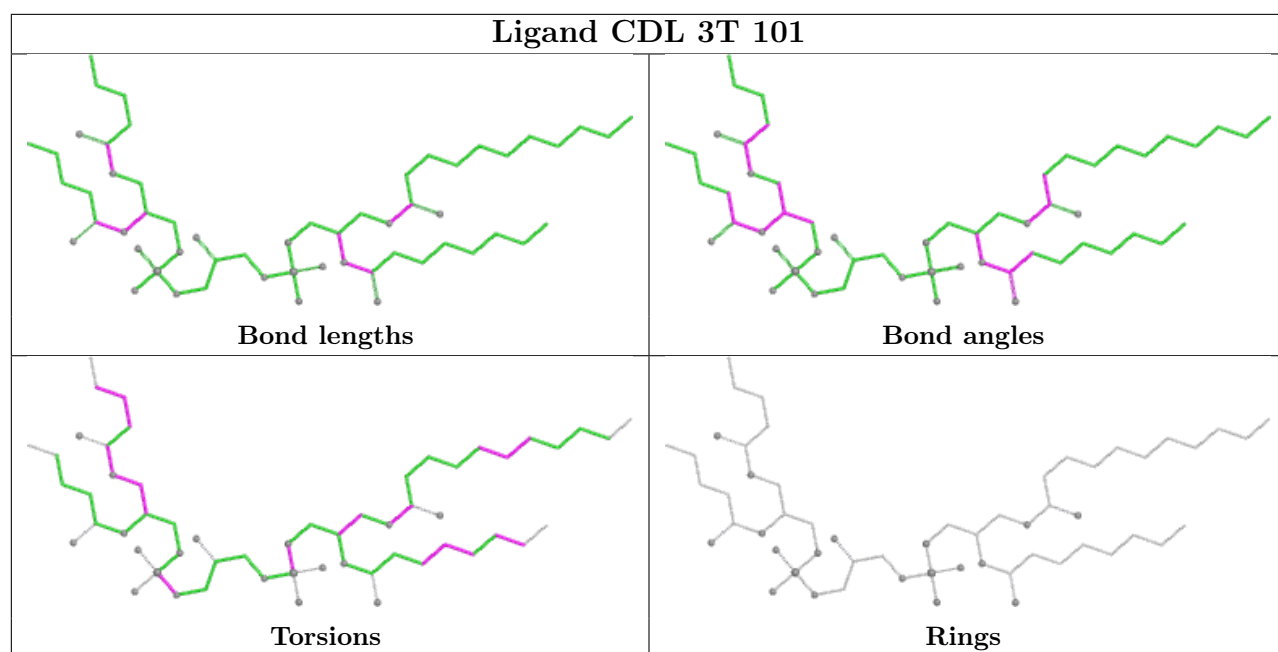


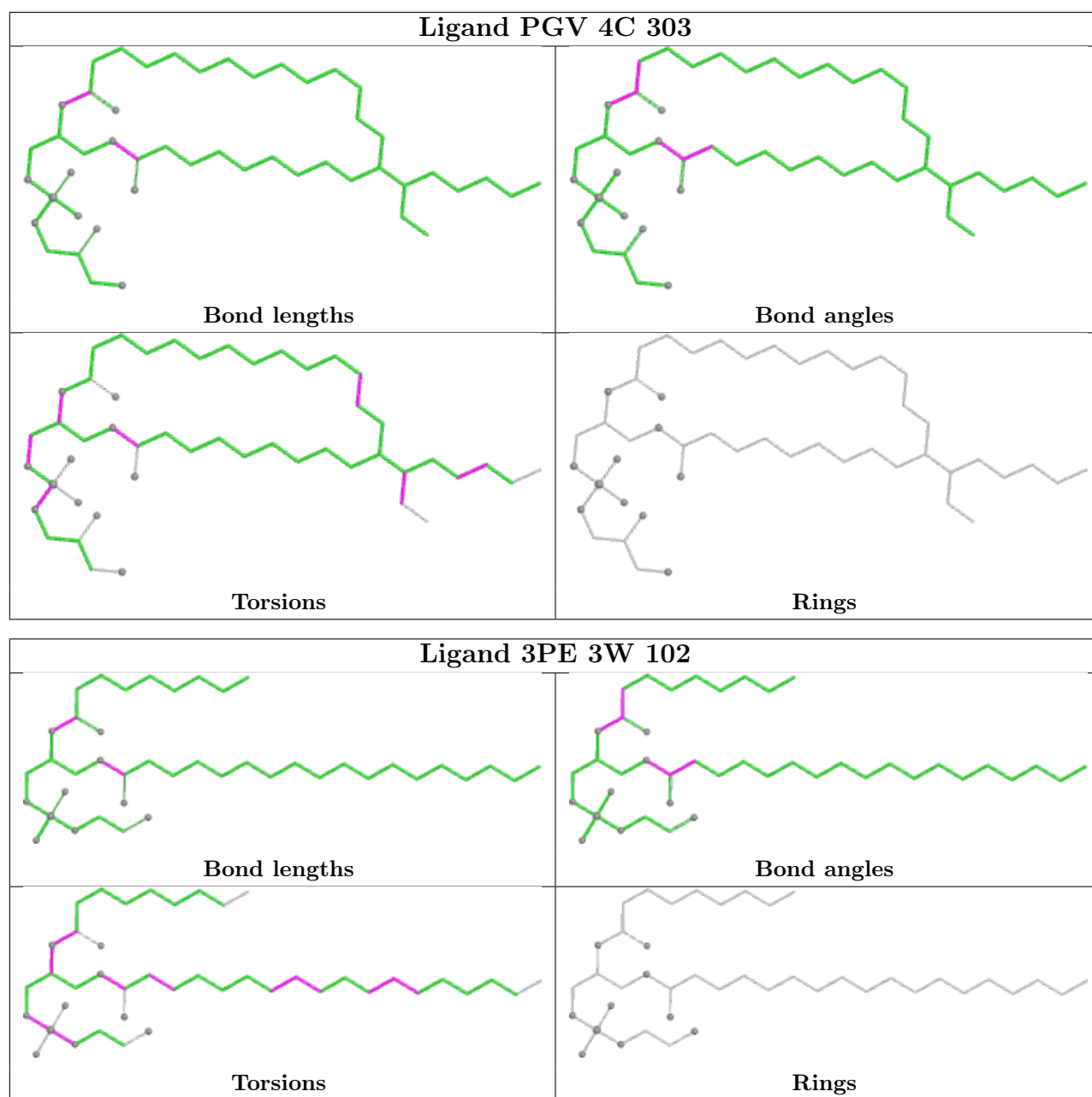


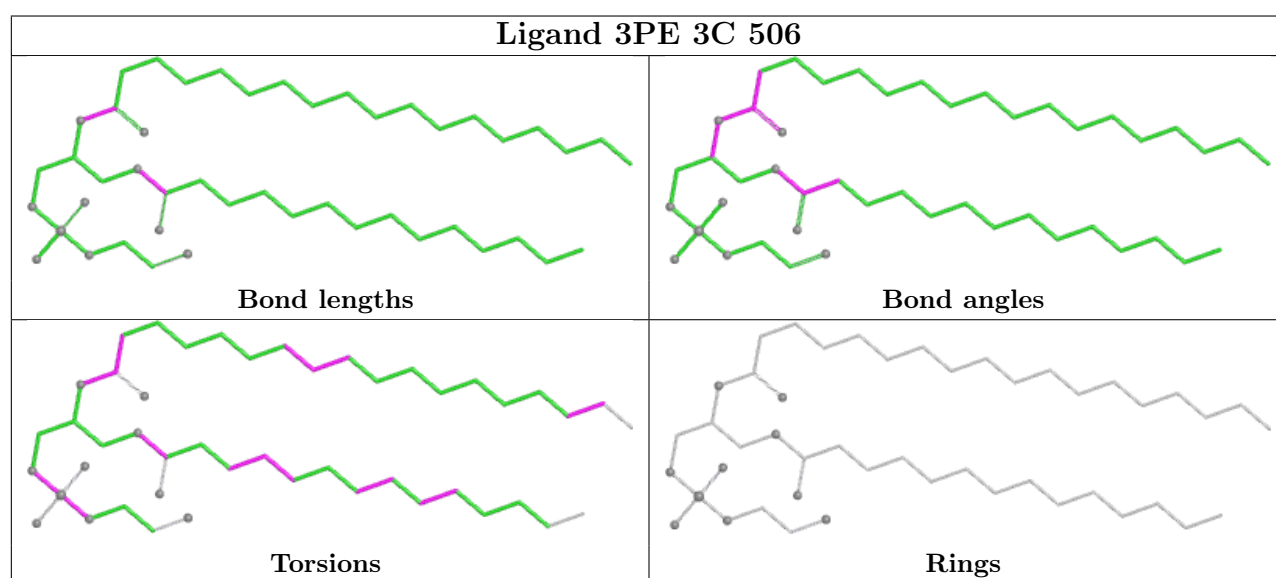
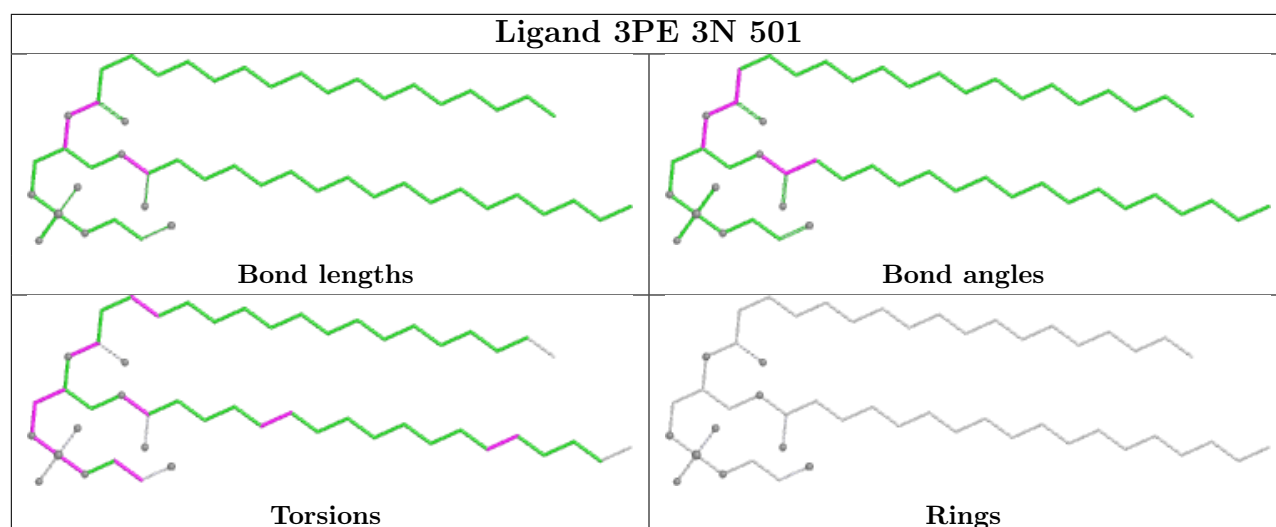


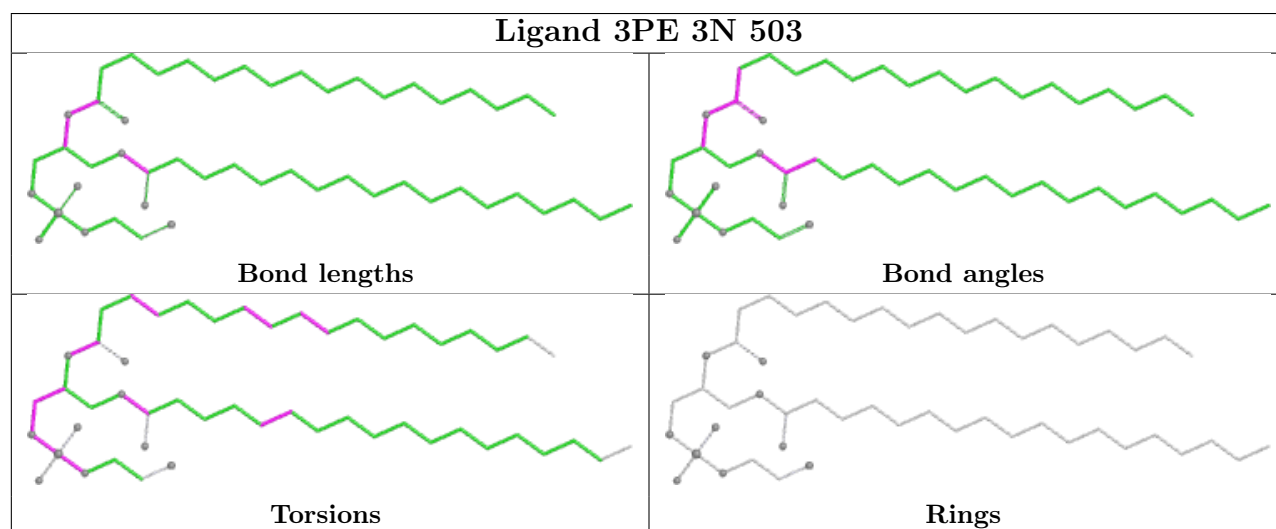
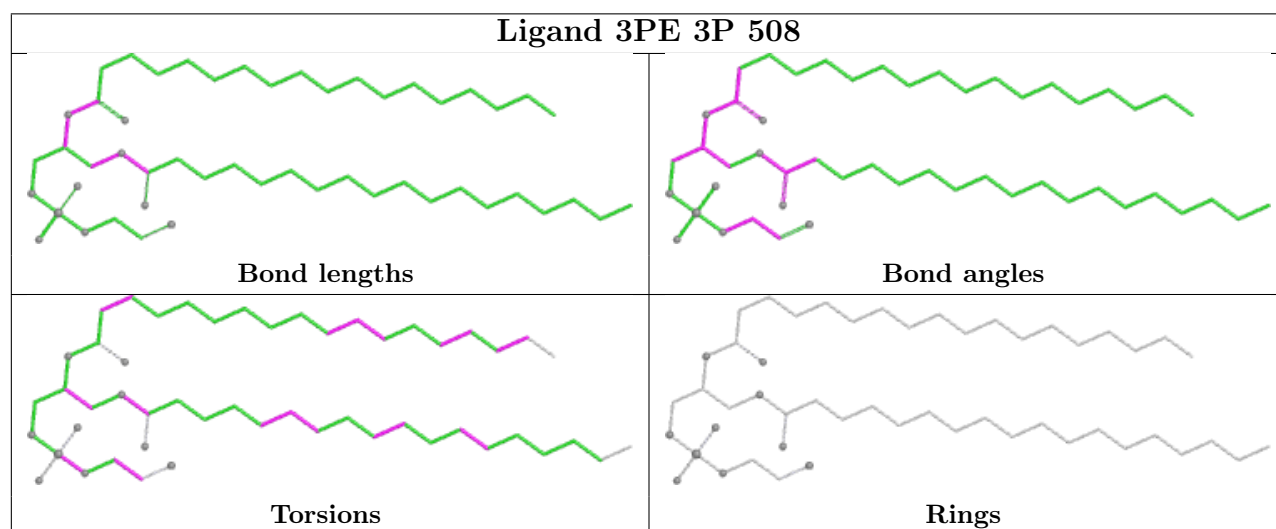
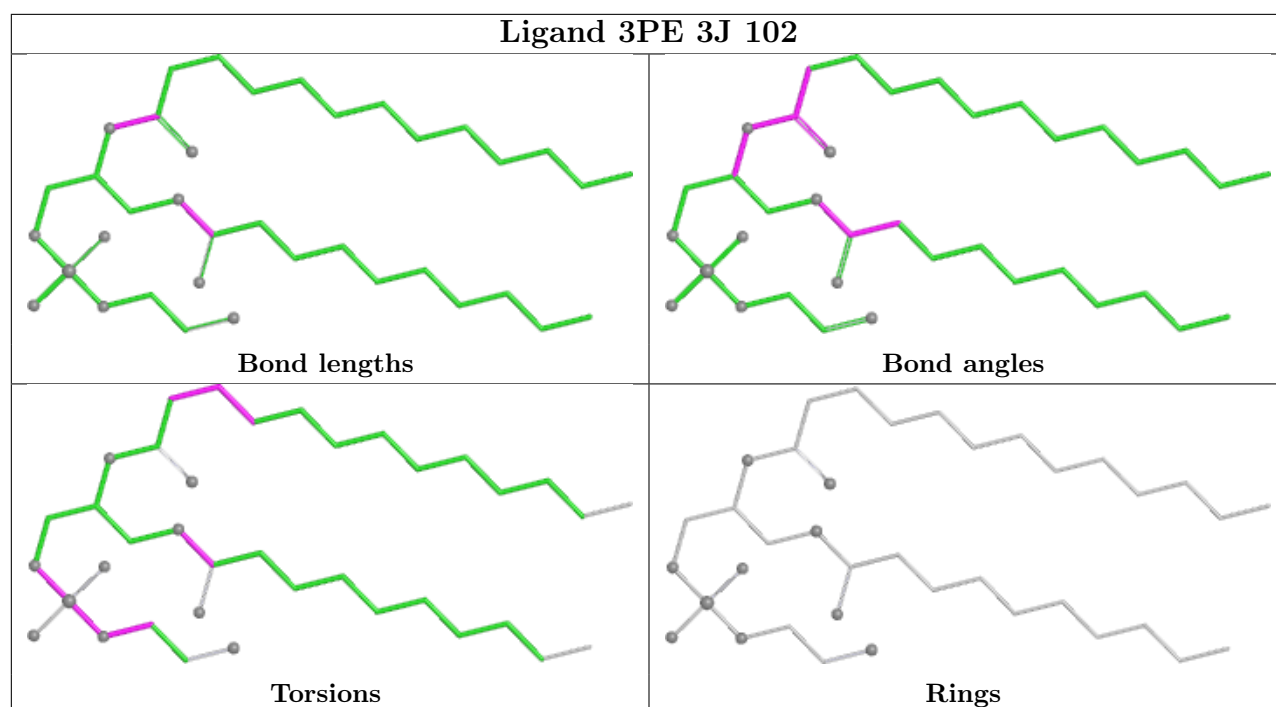


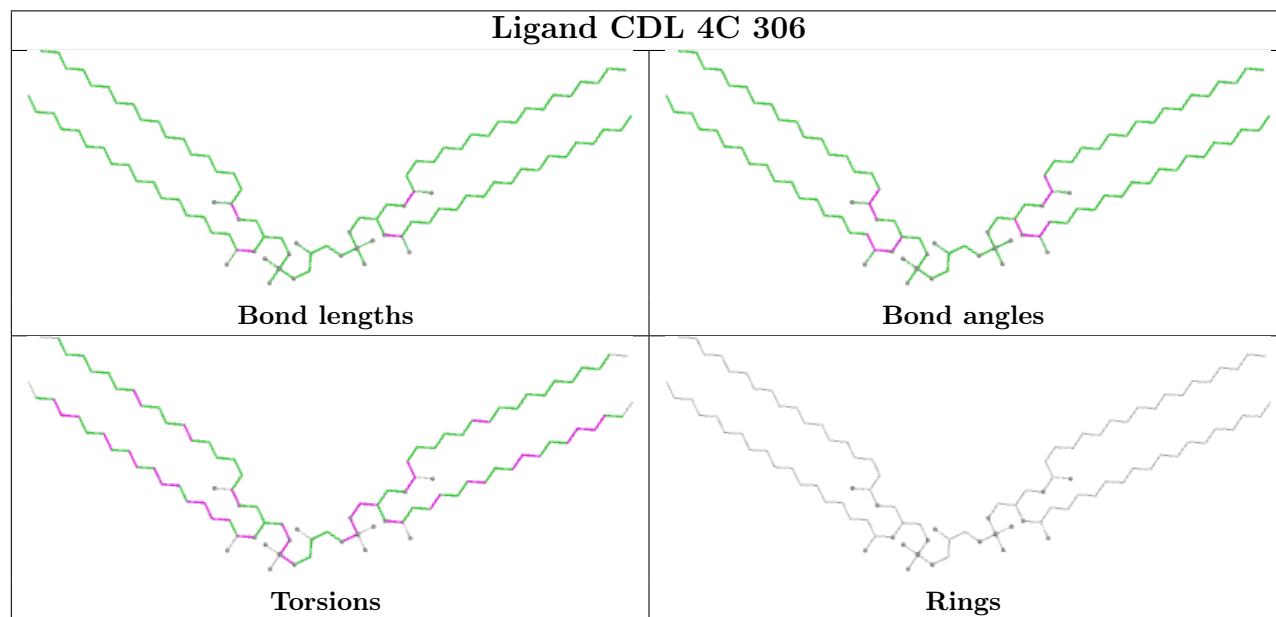
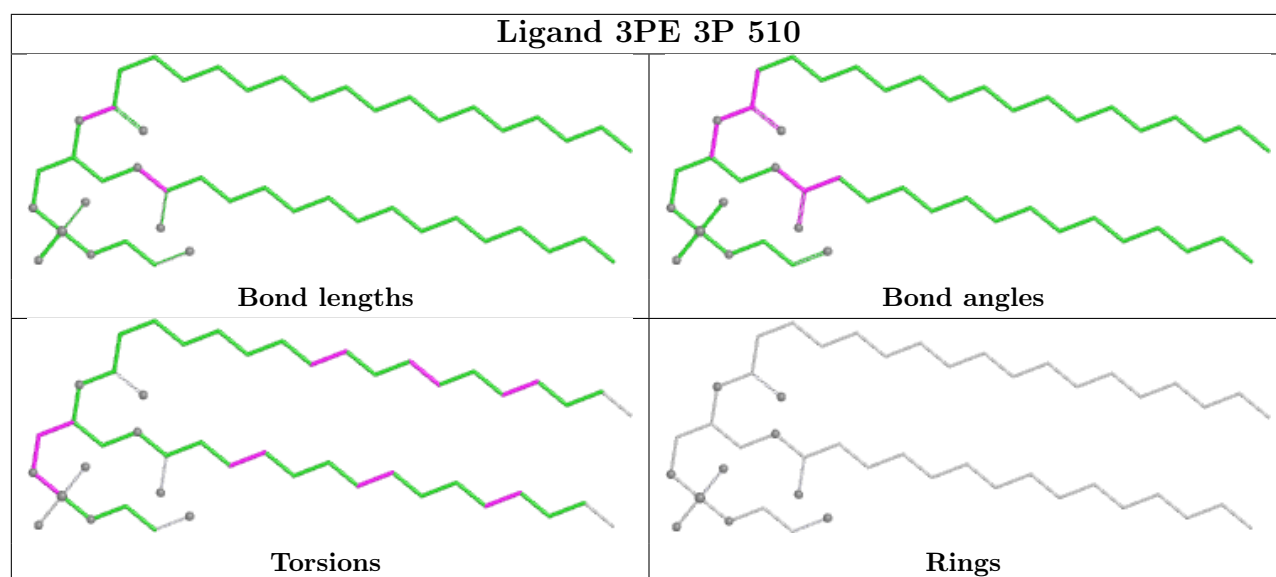


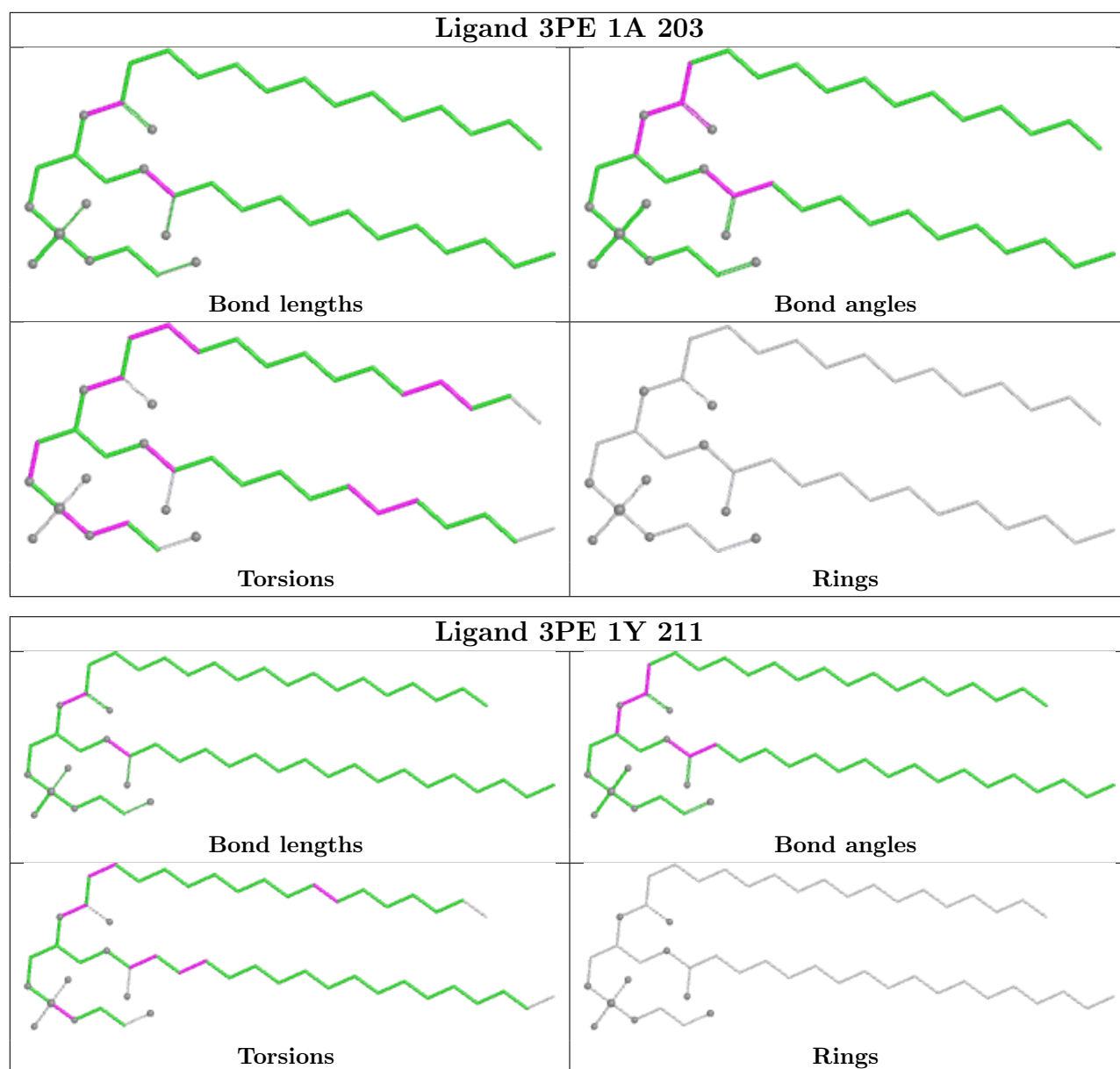


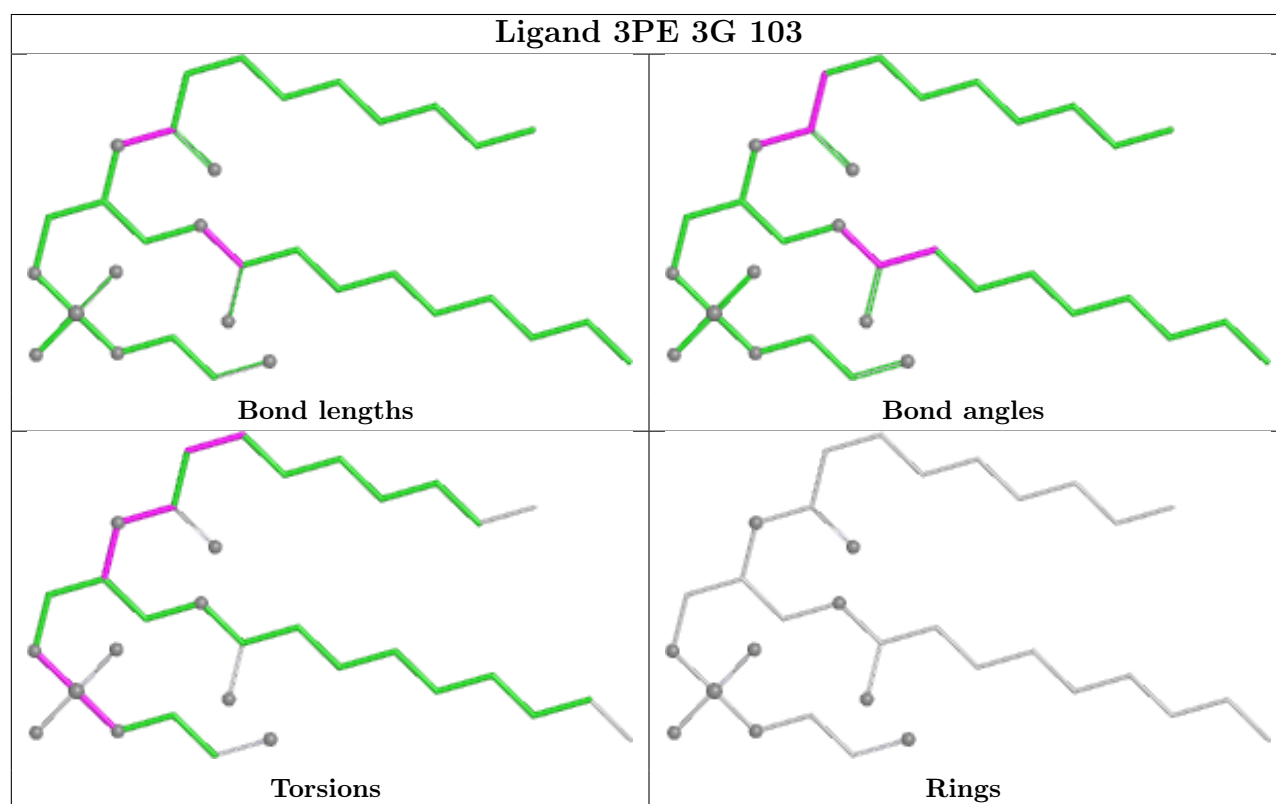
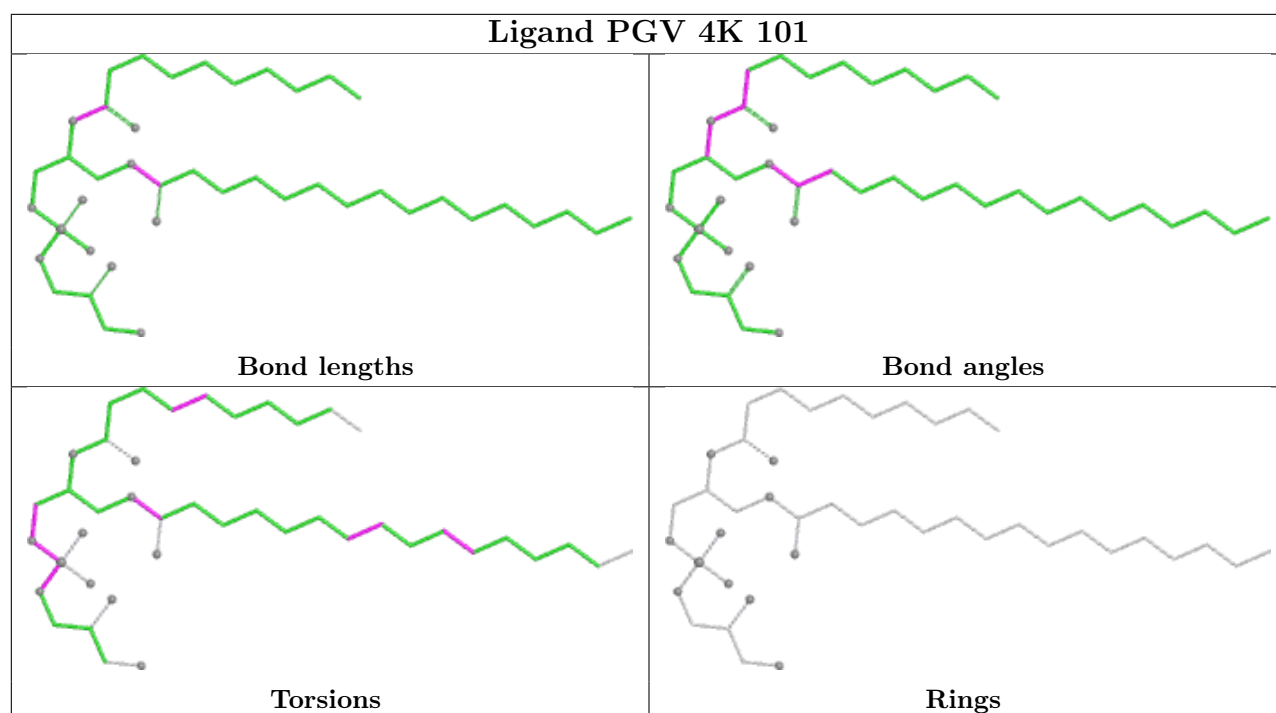


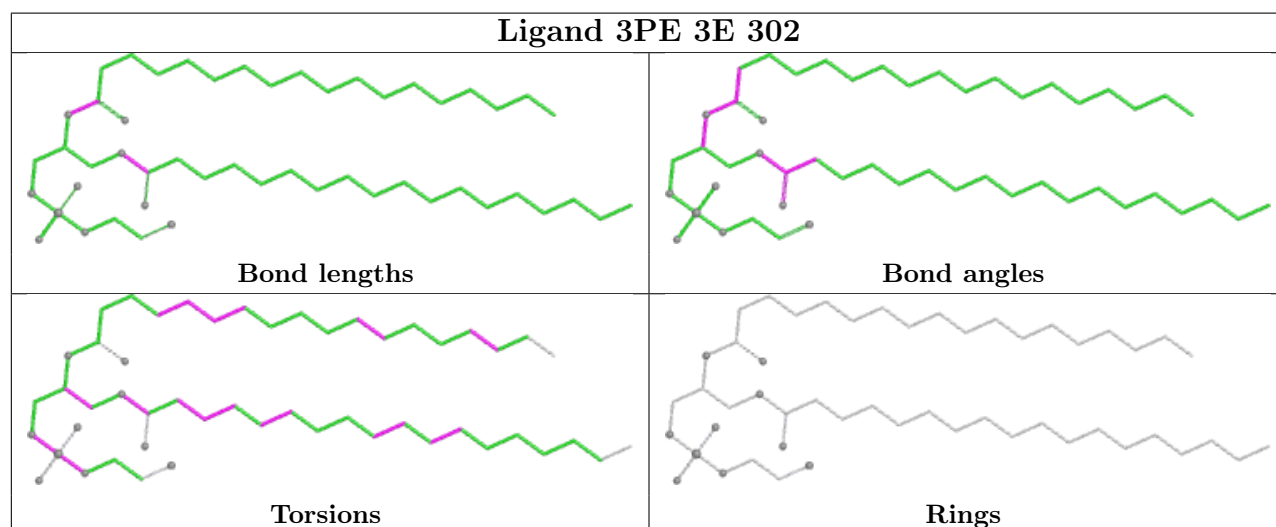
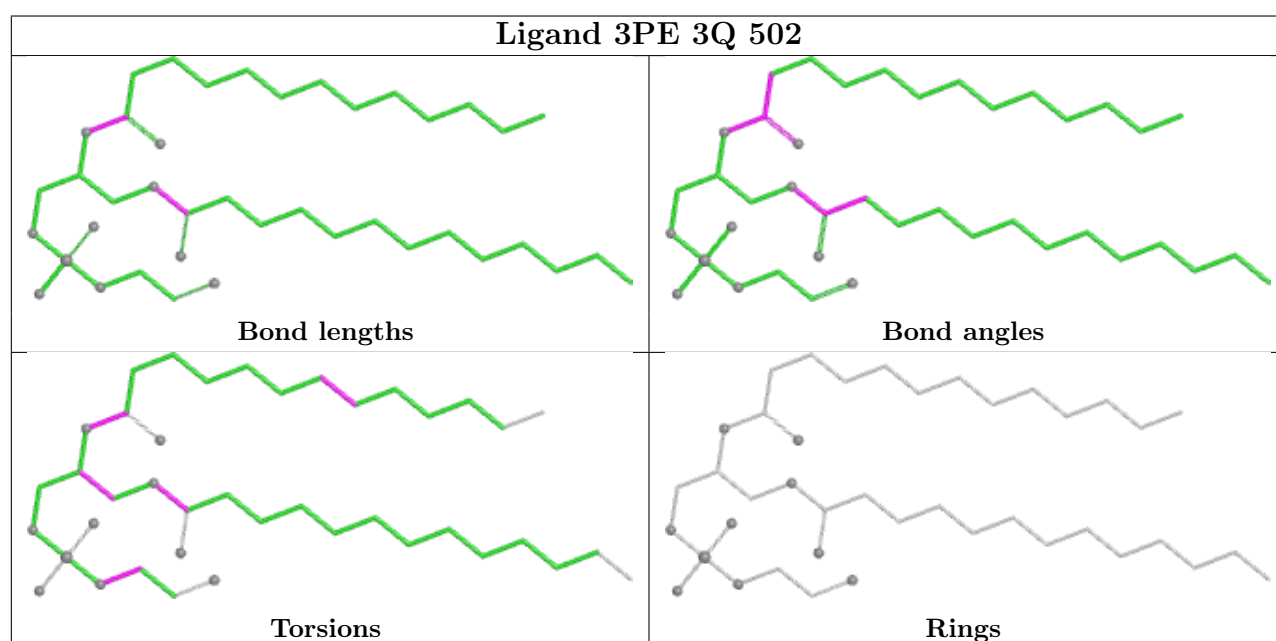
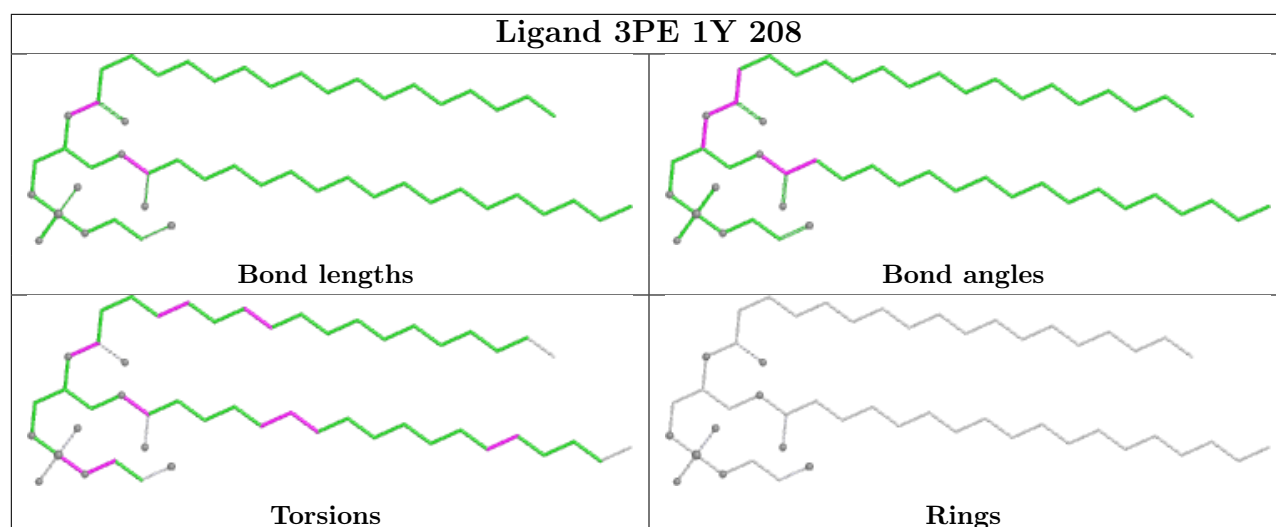


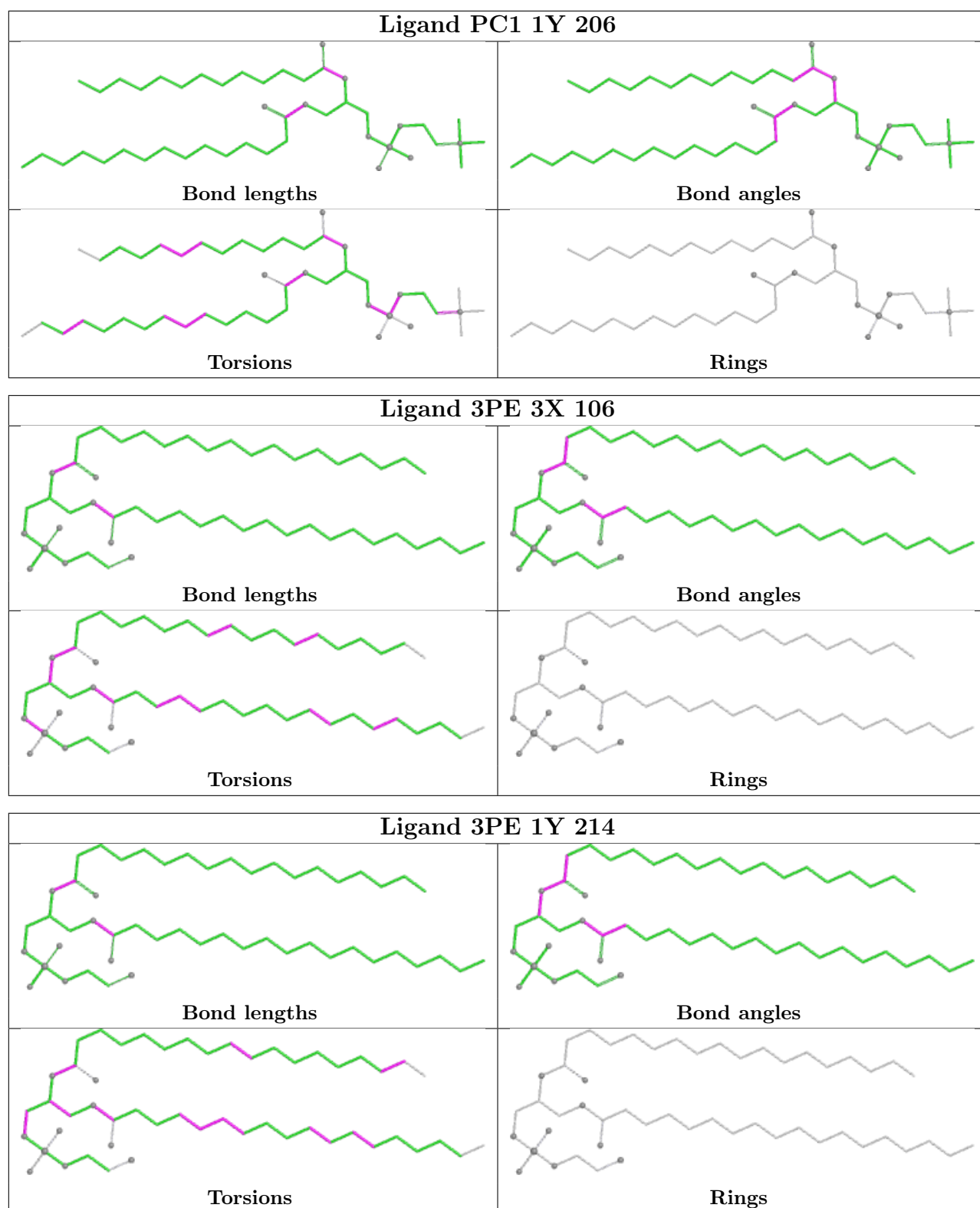


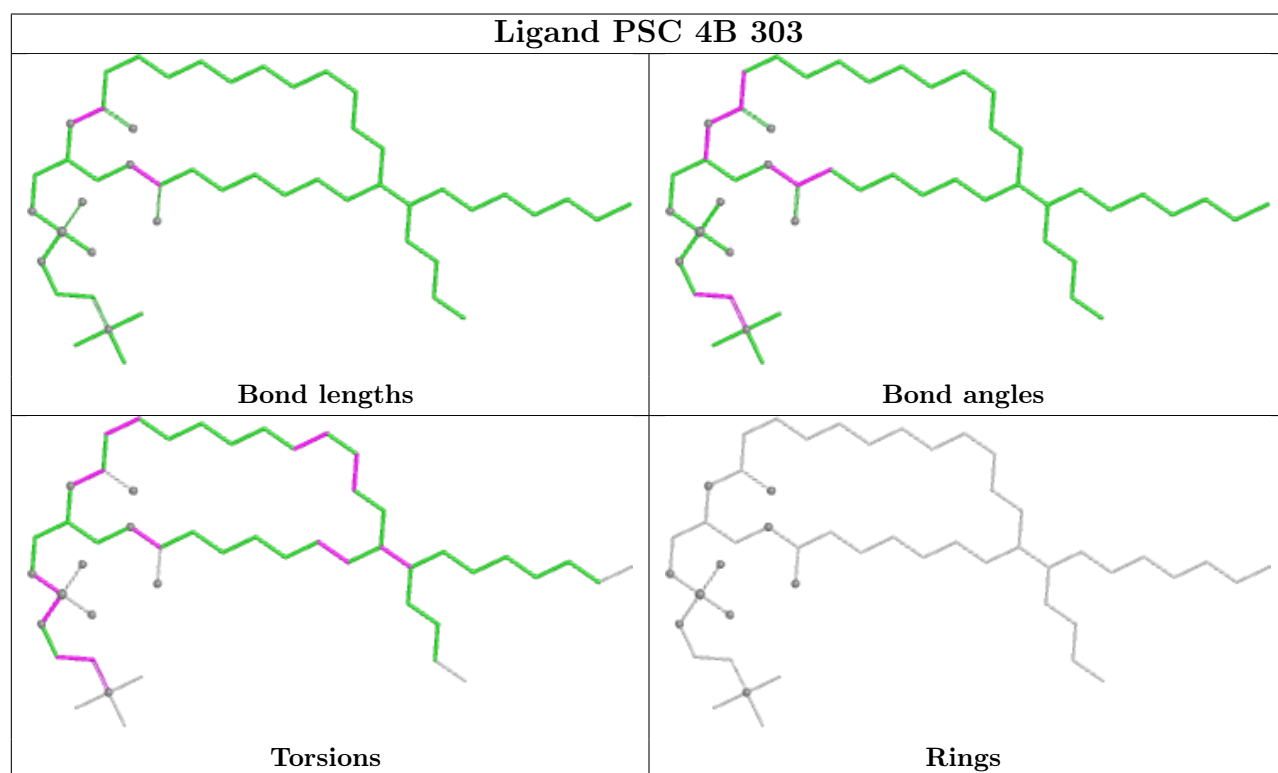
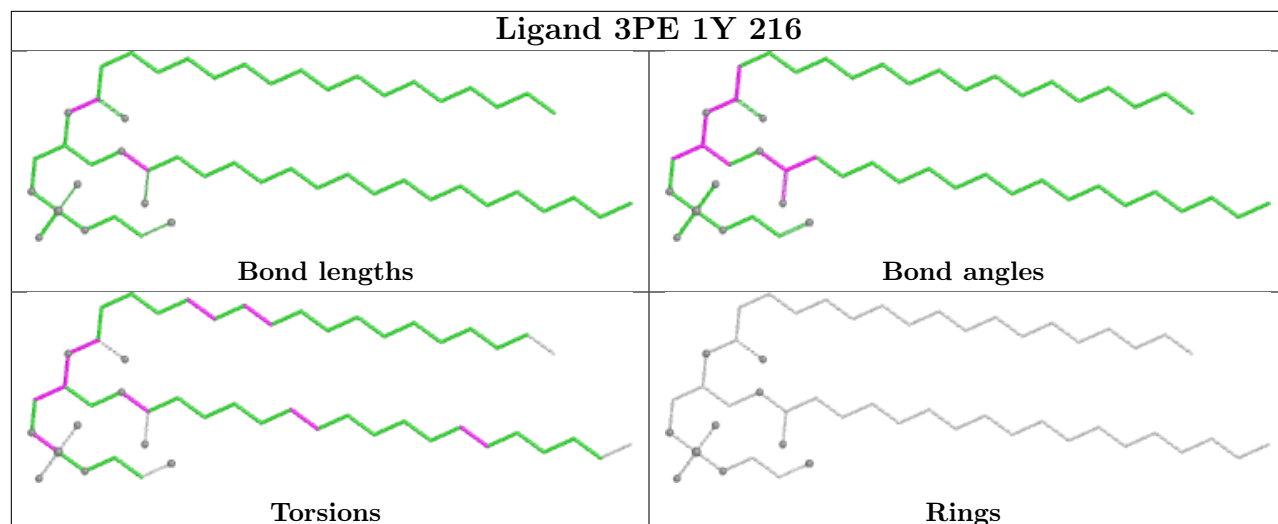


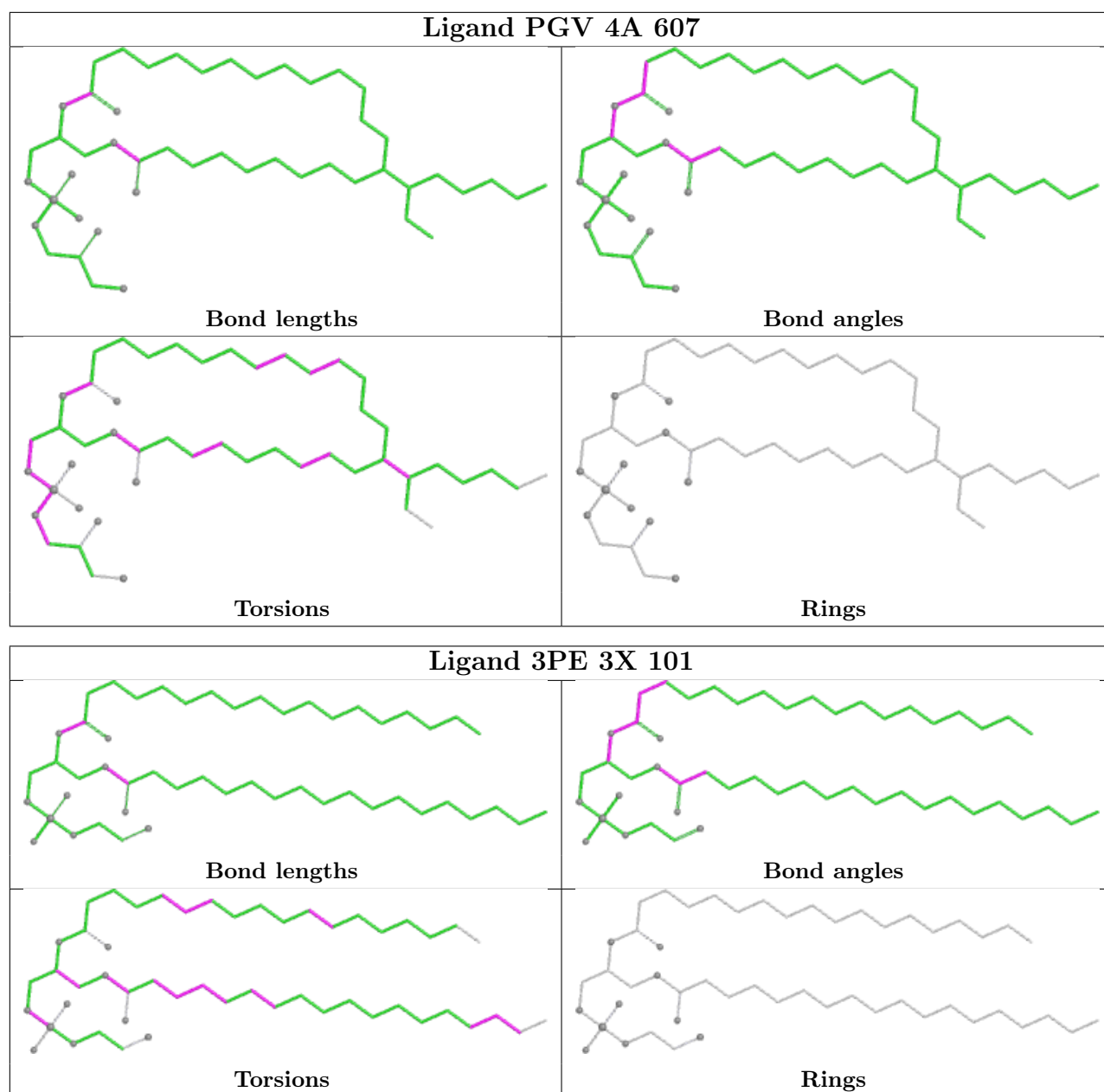




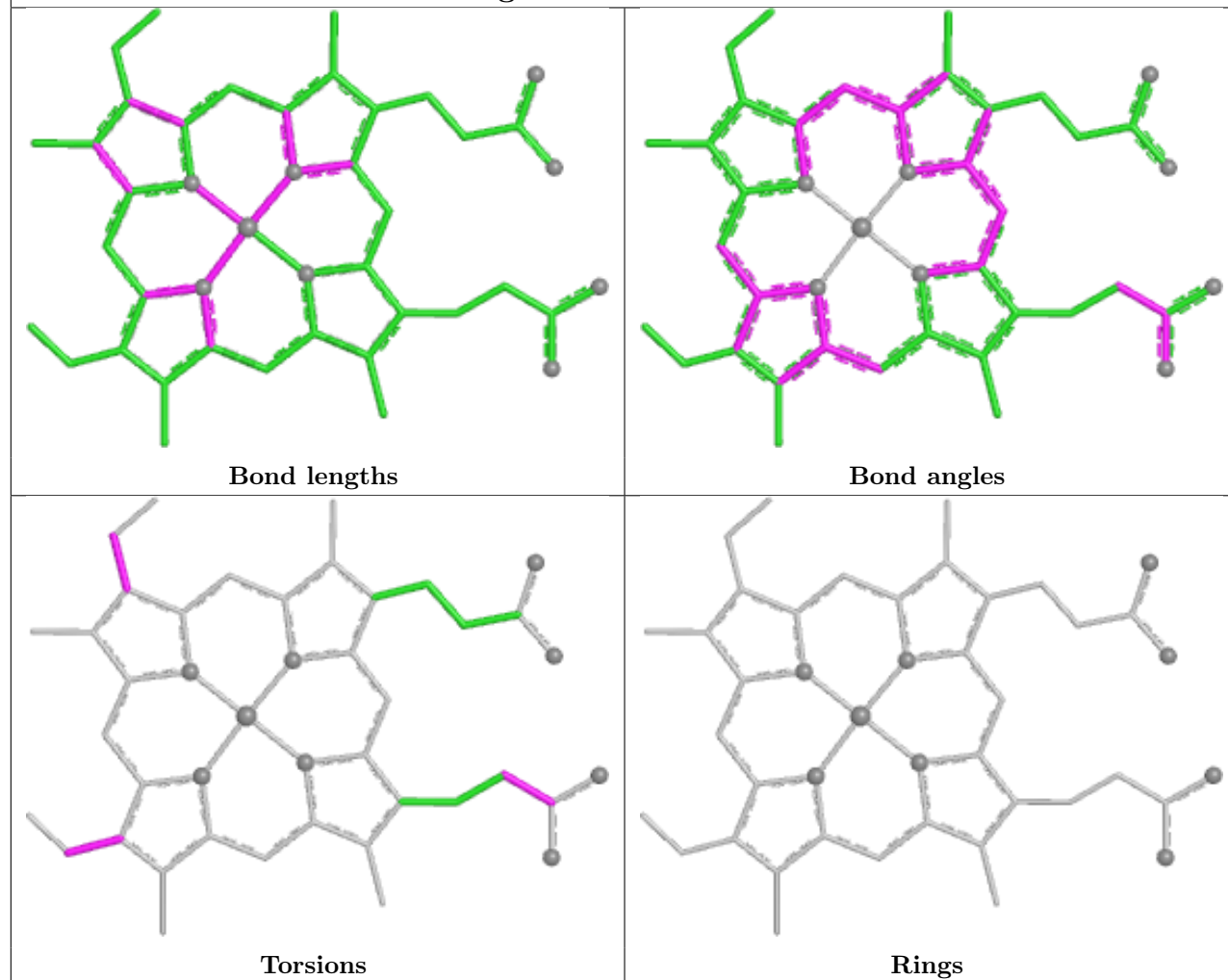




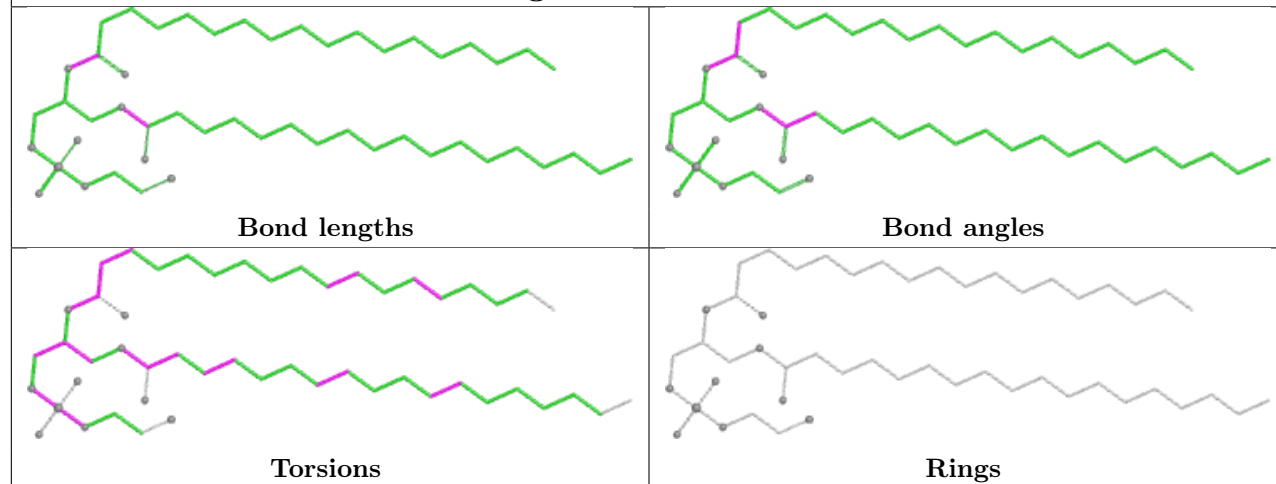


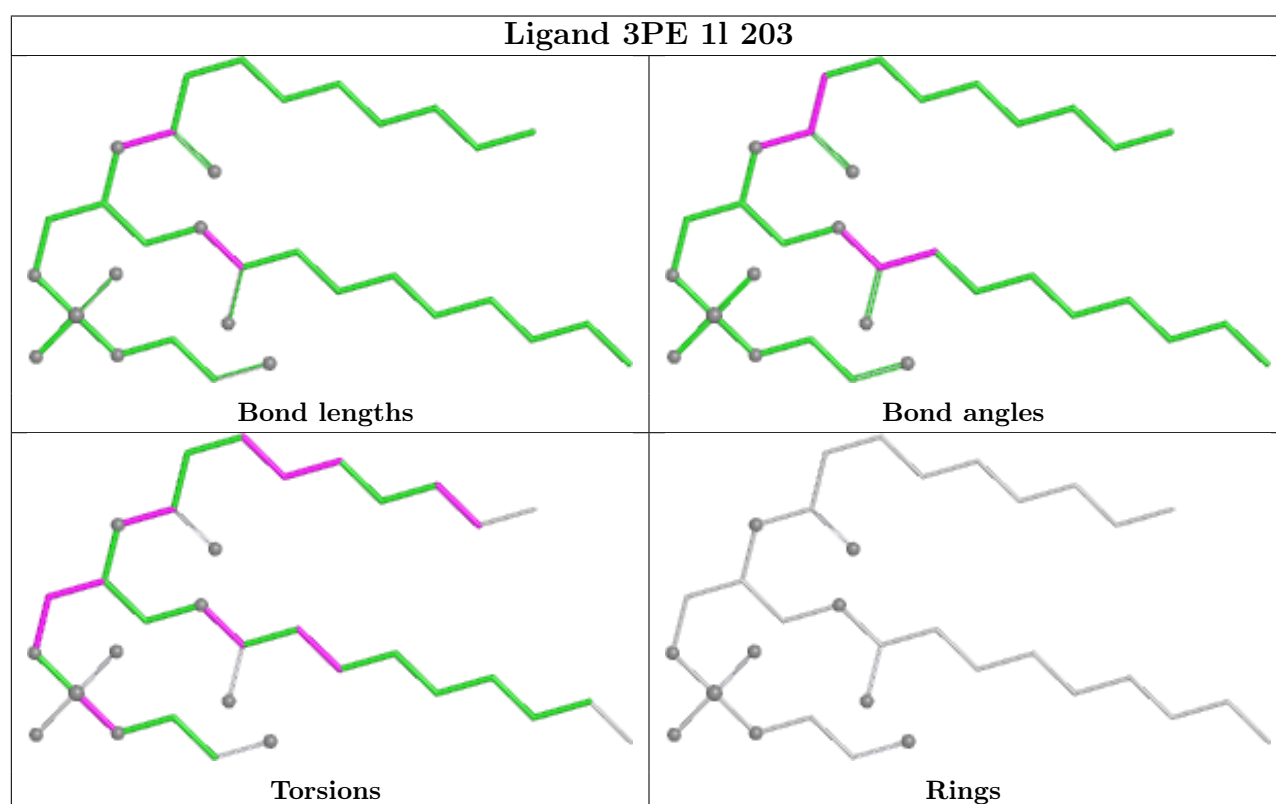
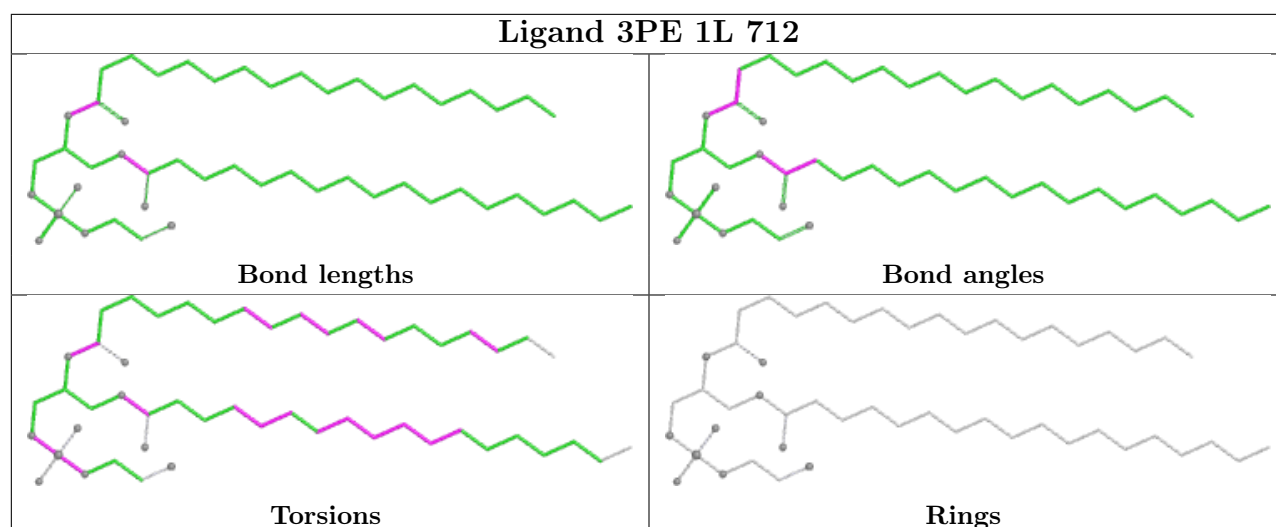


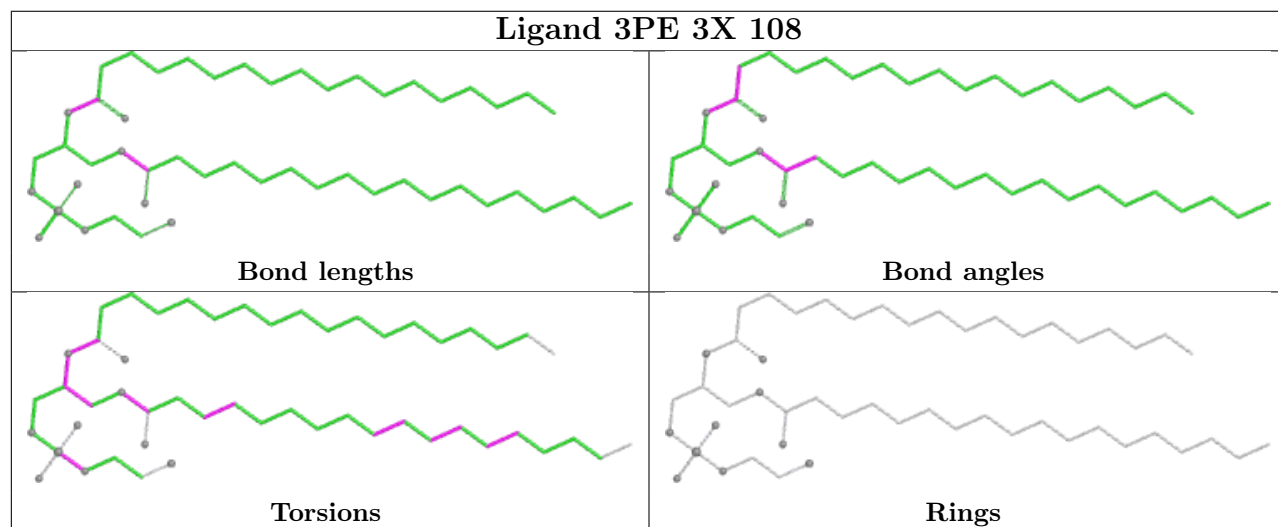
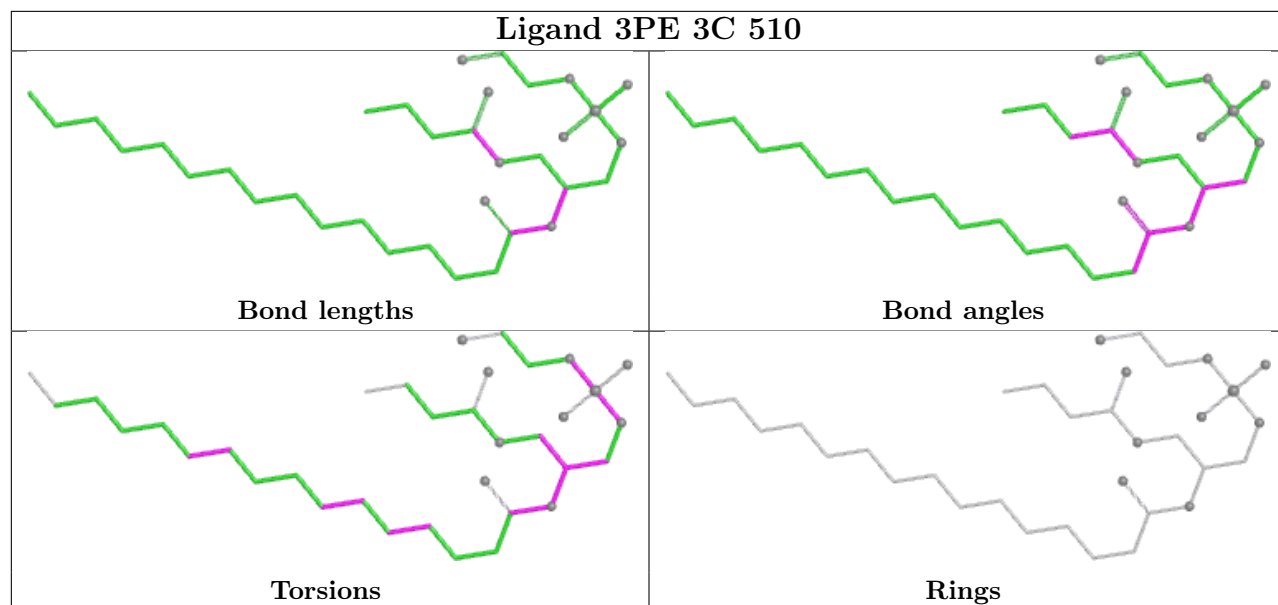
Ligand HEM 3C 502

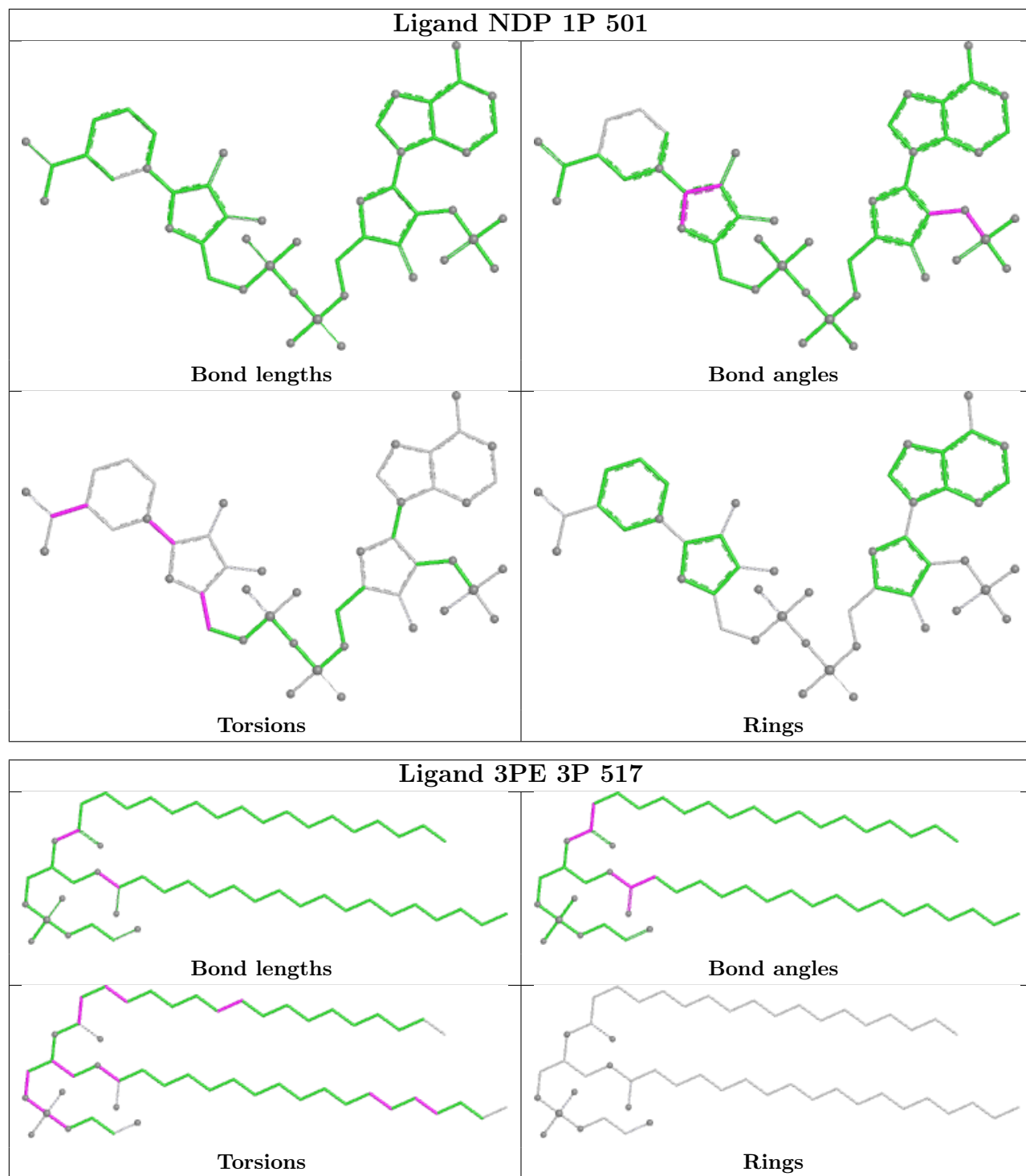


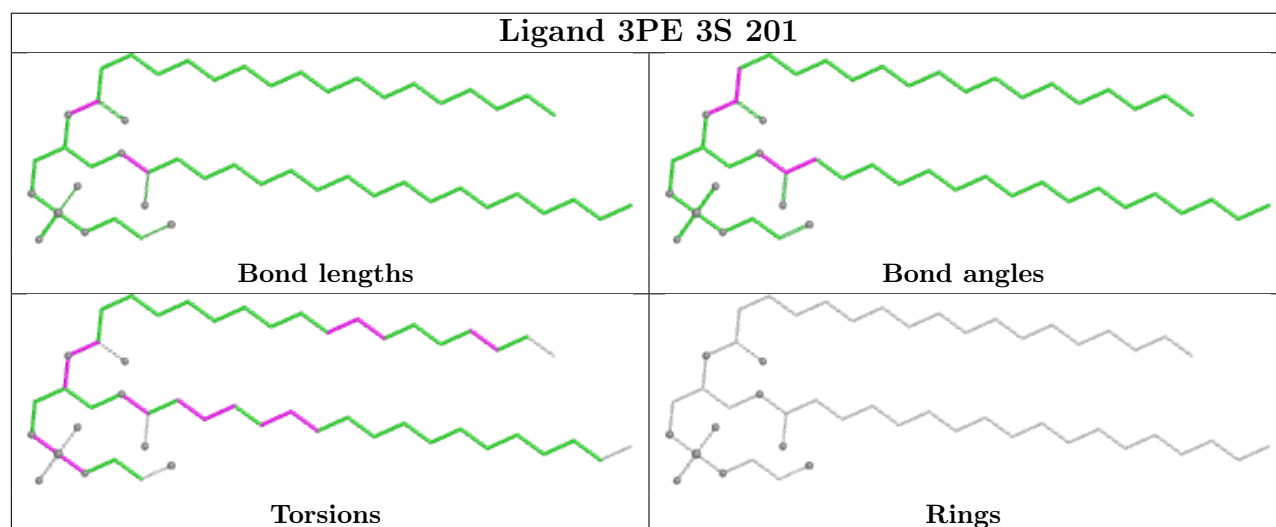
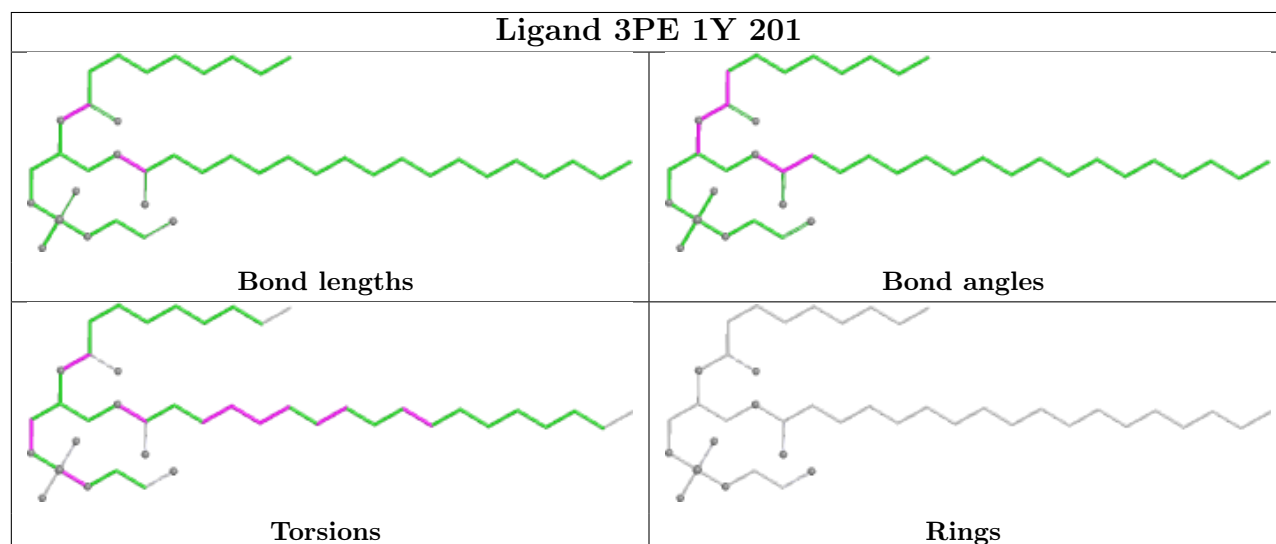
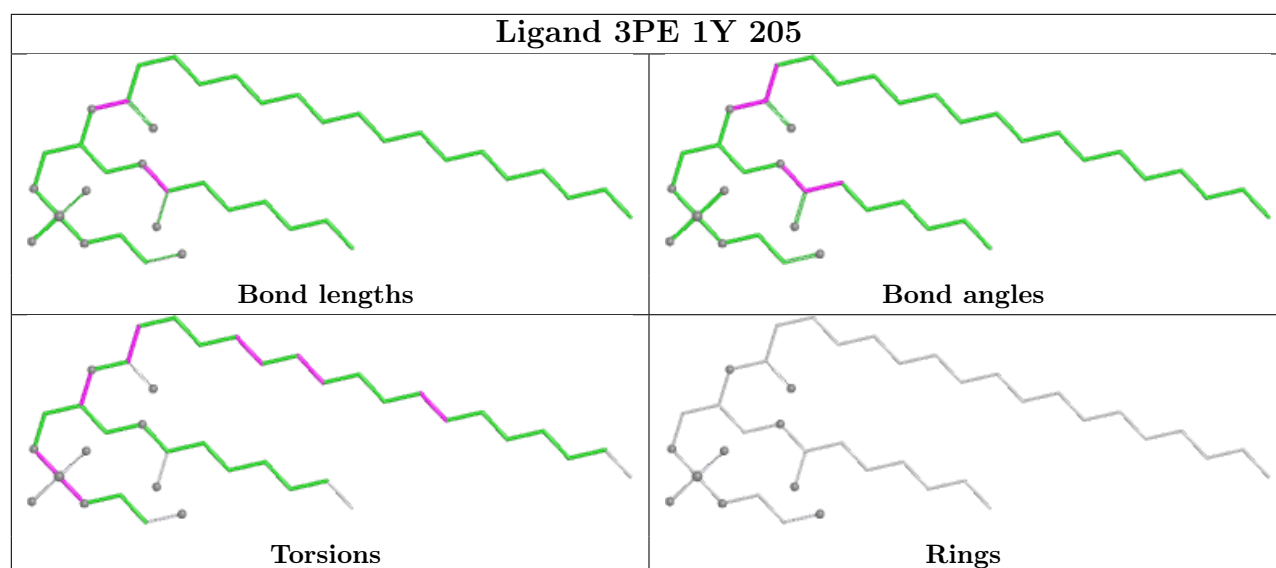
Ligand 3PE 3C 507



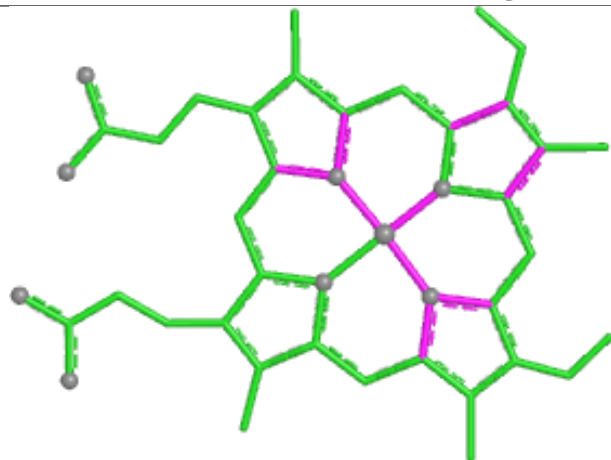




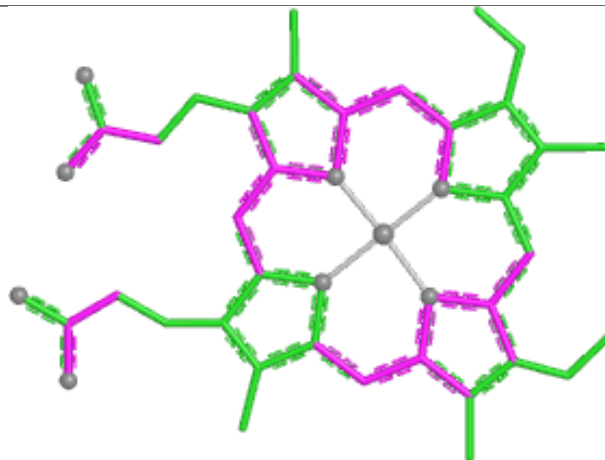




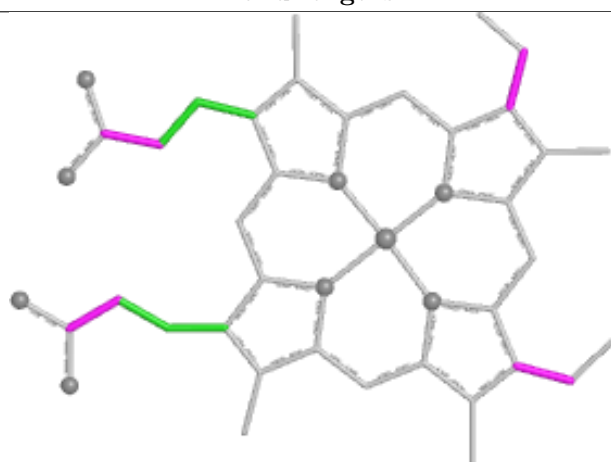
Ligand HEM 3P 502



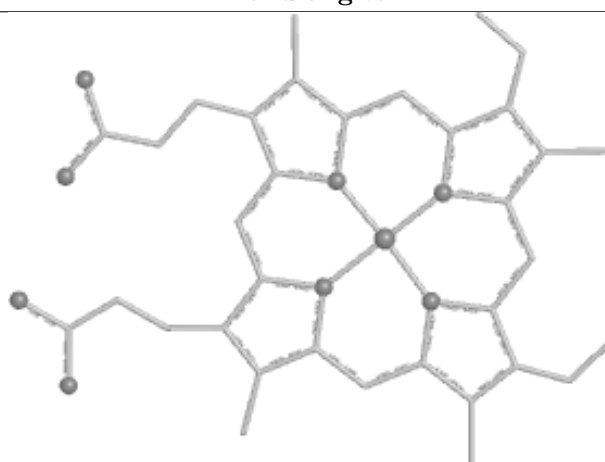
Bond lengths



Bond angles

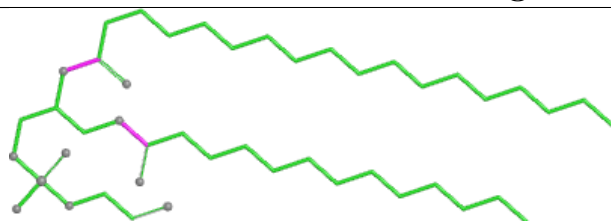


Torsions

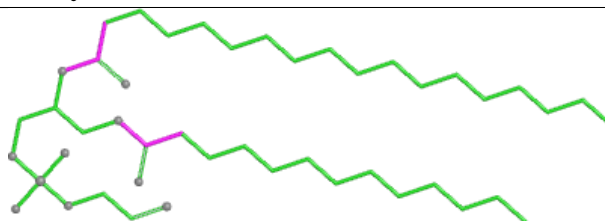


Rings

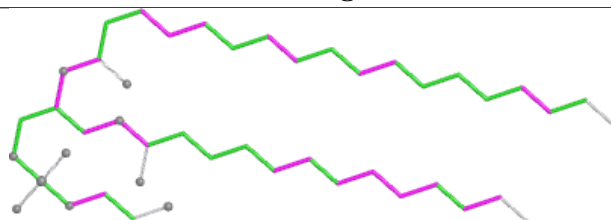
Ligand 3PE 3Q 503



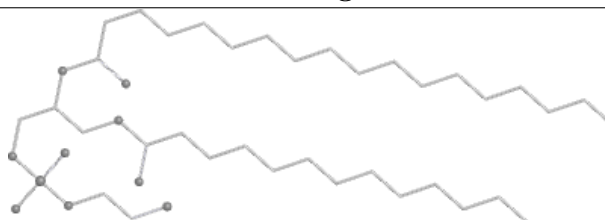
Bond lengths



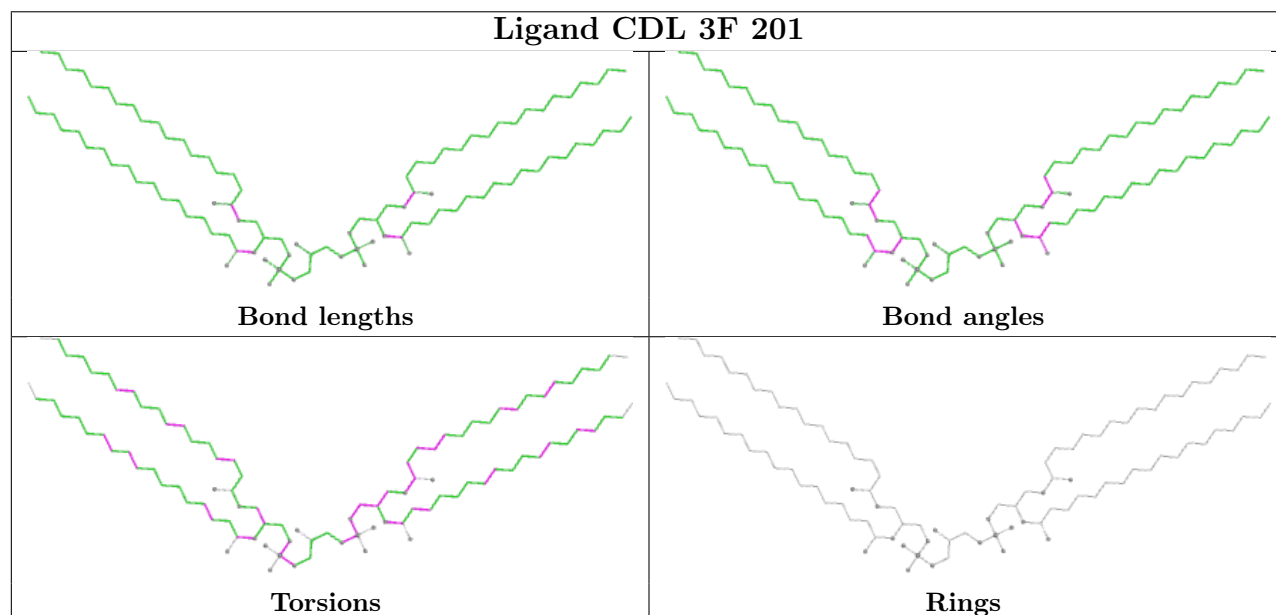
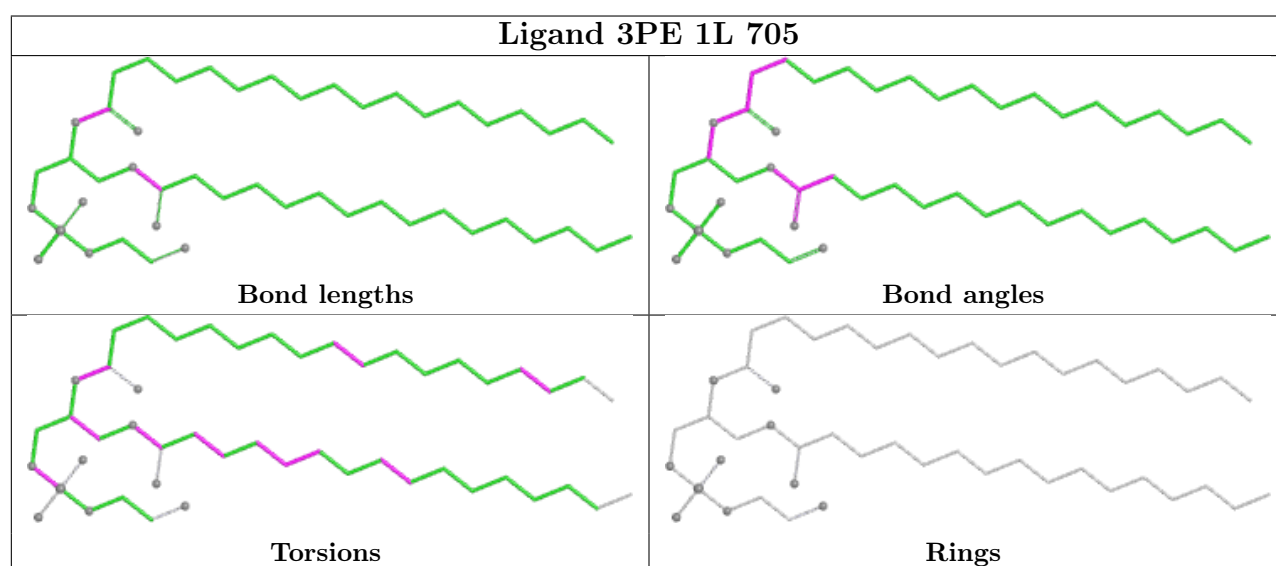
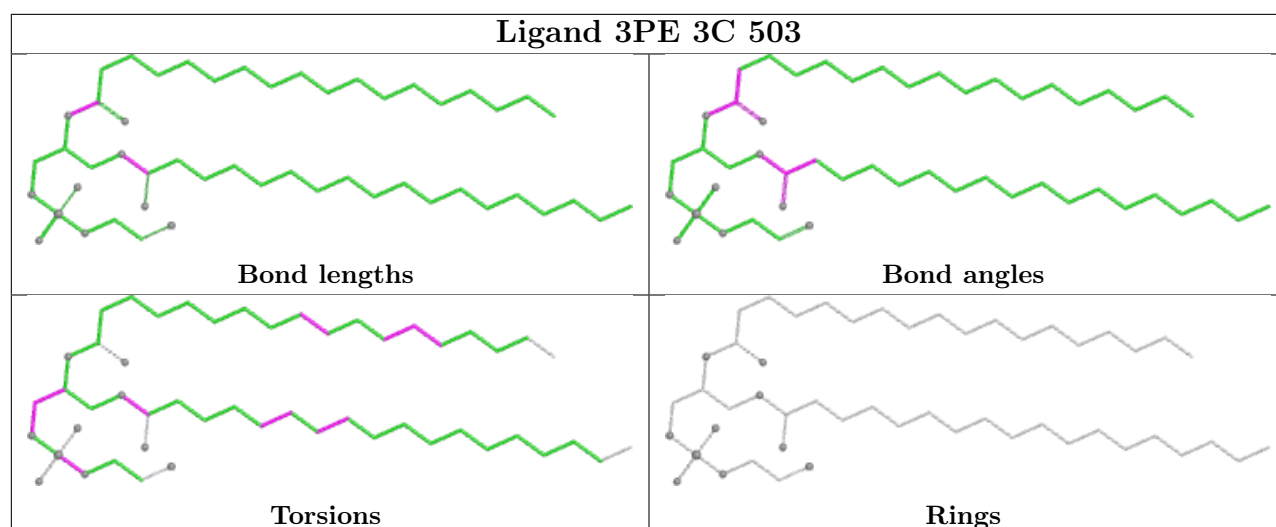
Bond angles



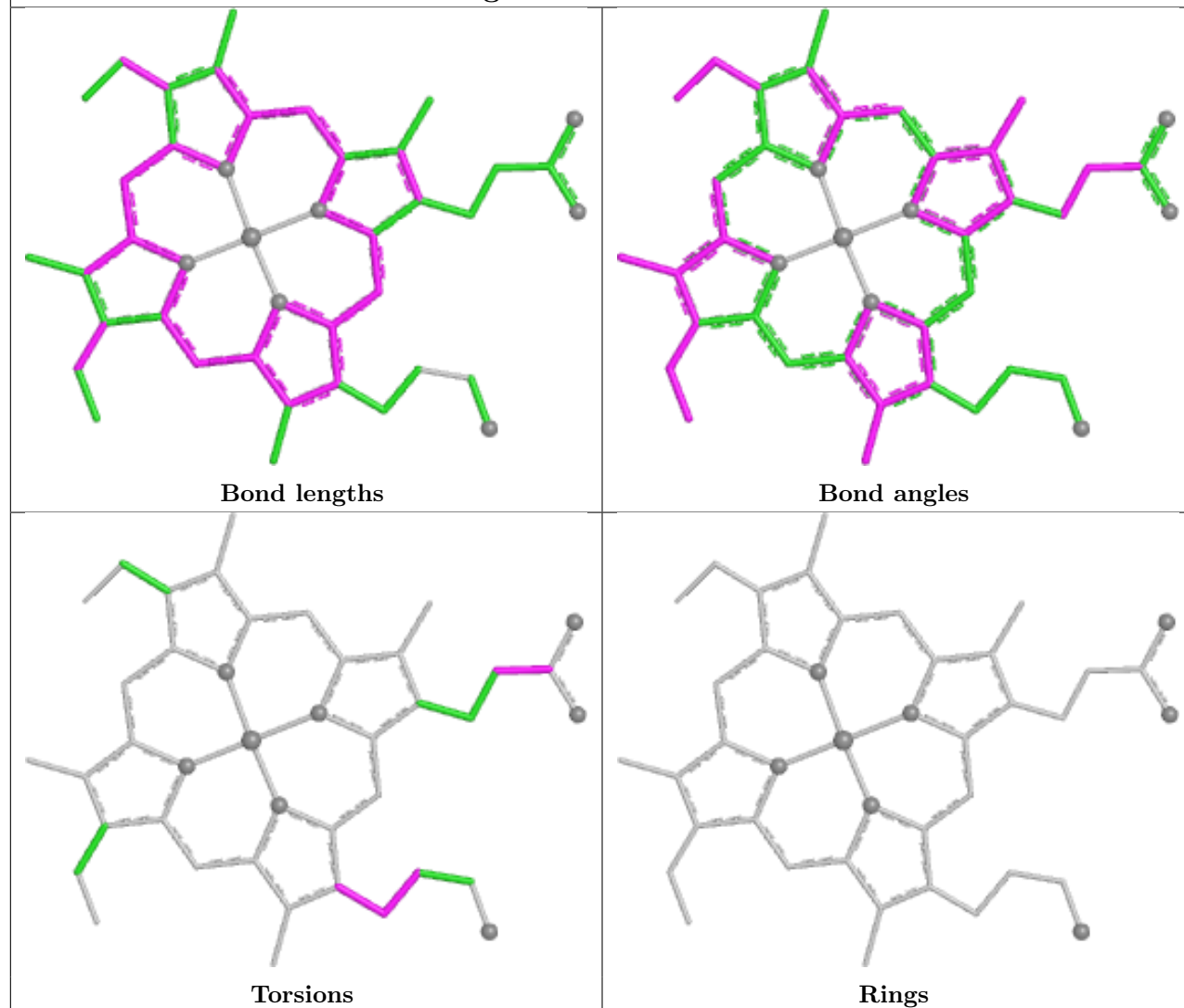
Torsions



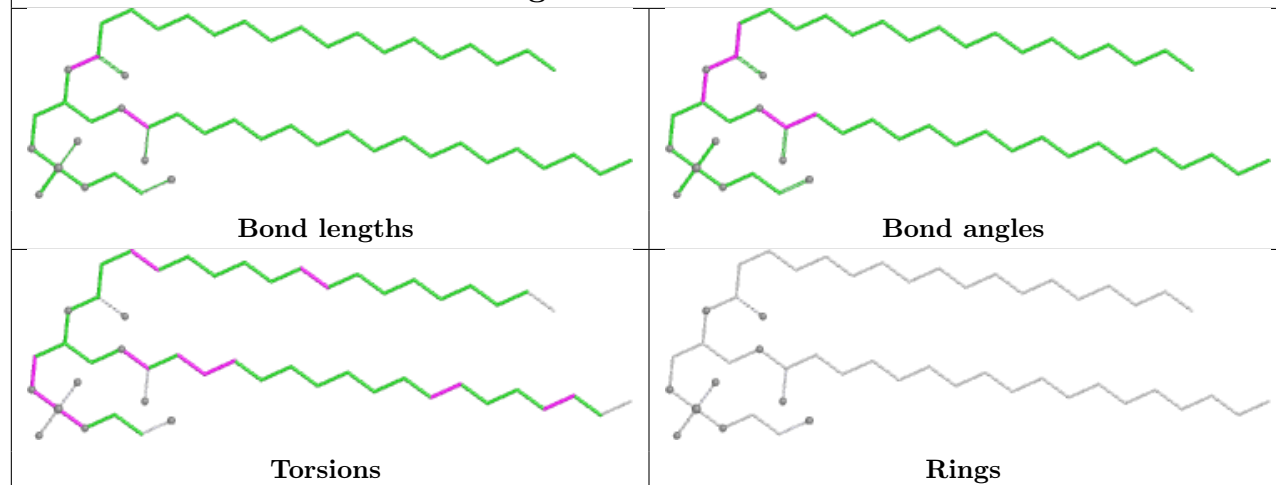
Rings

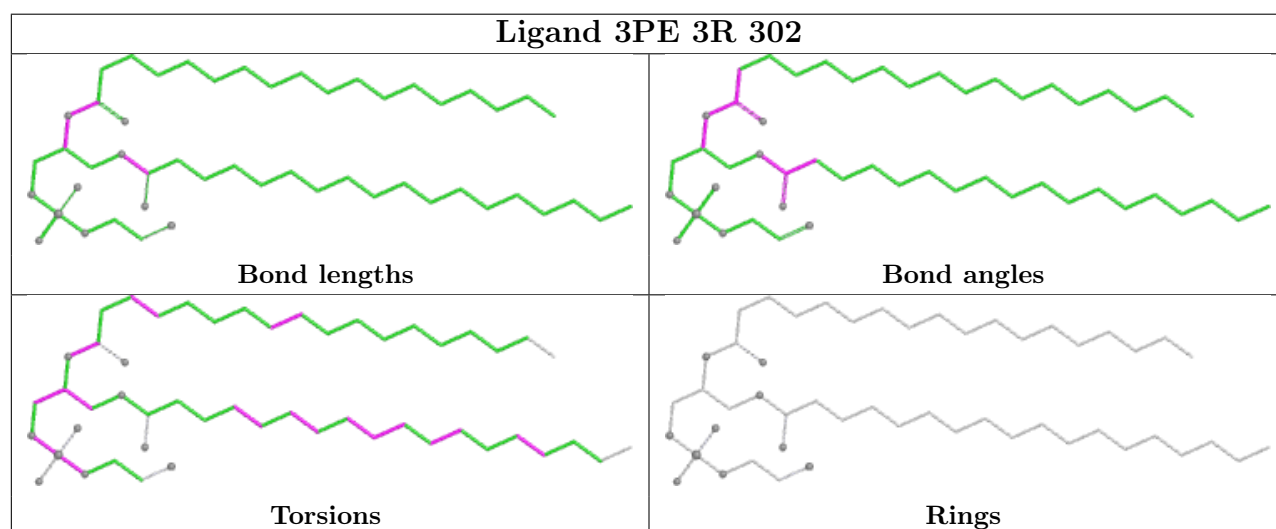
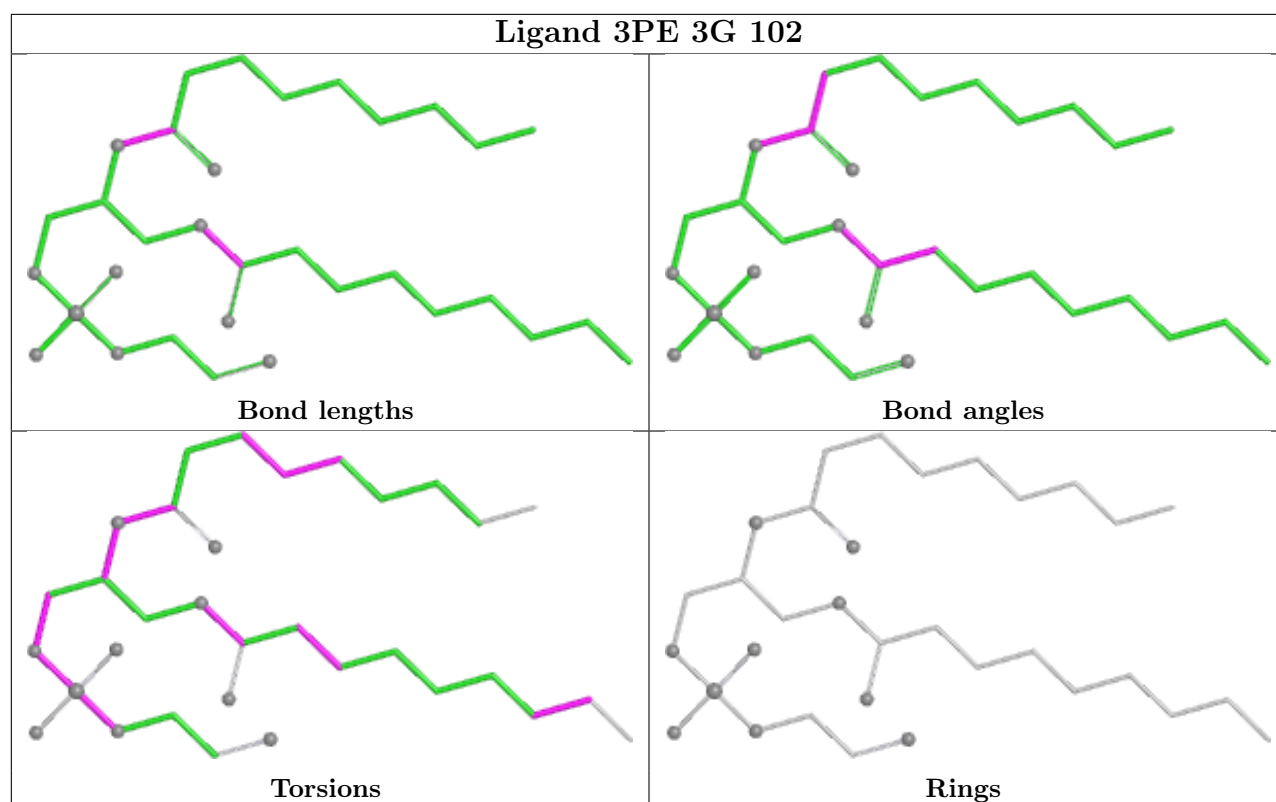


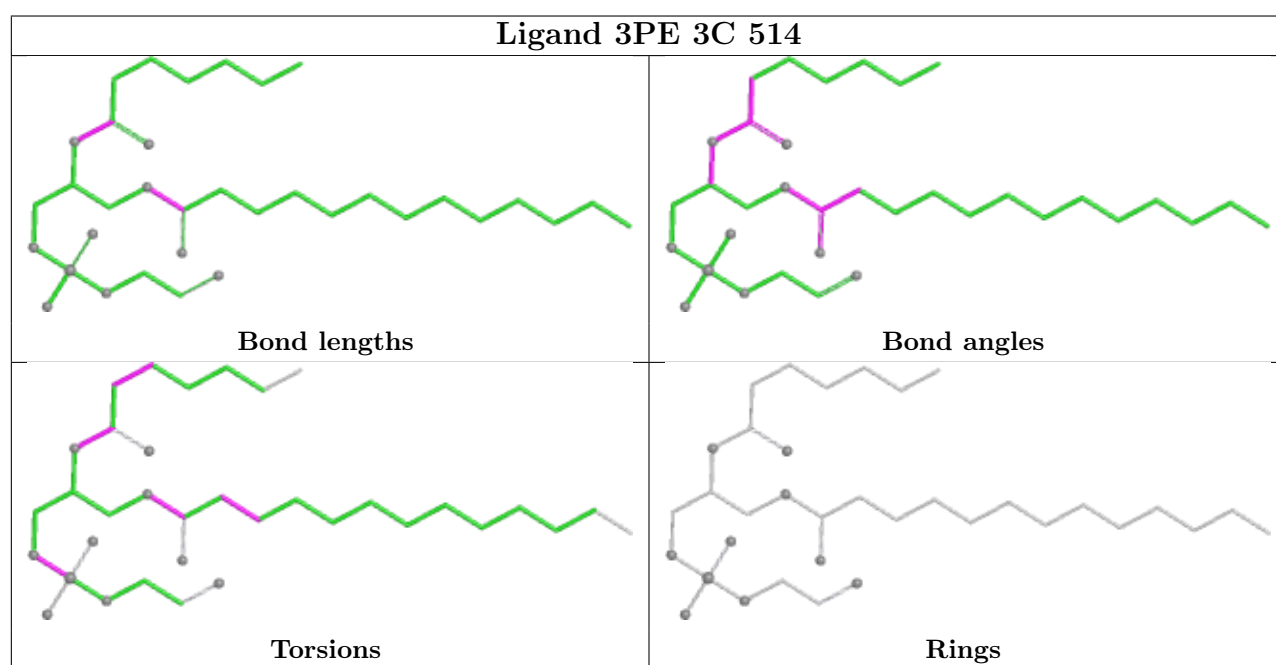
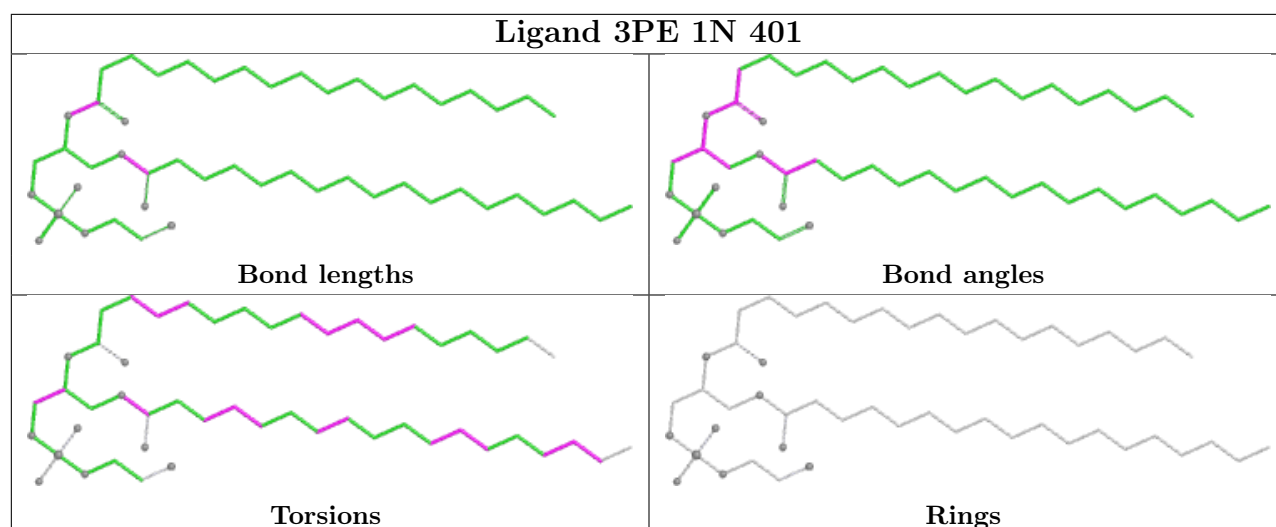
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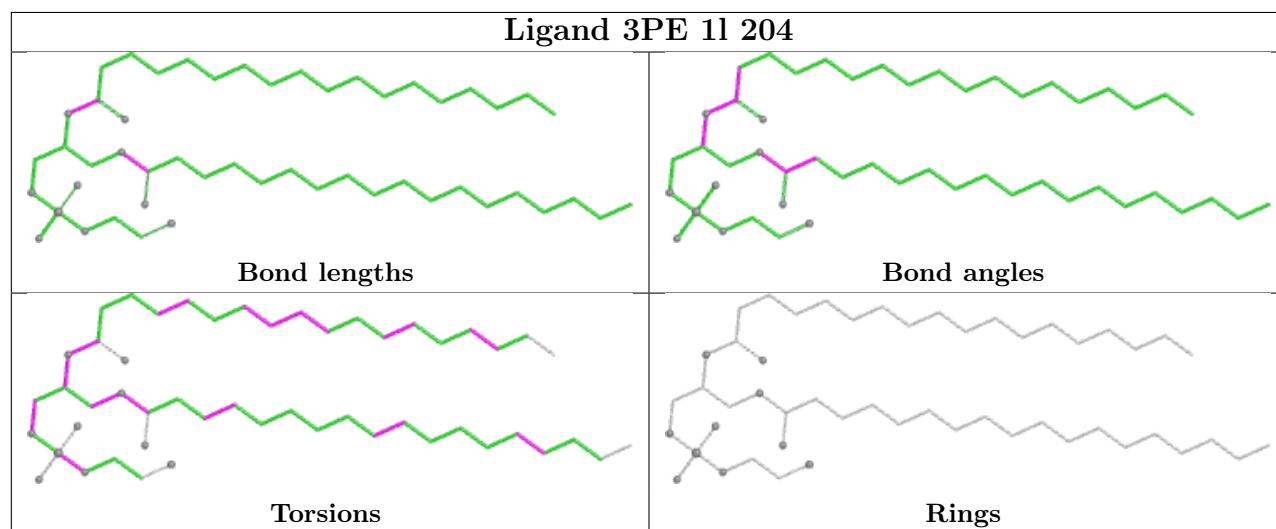
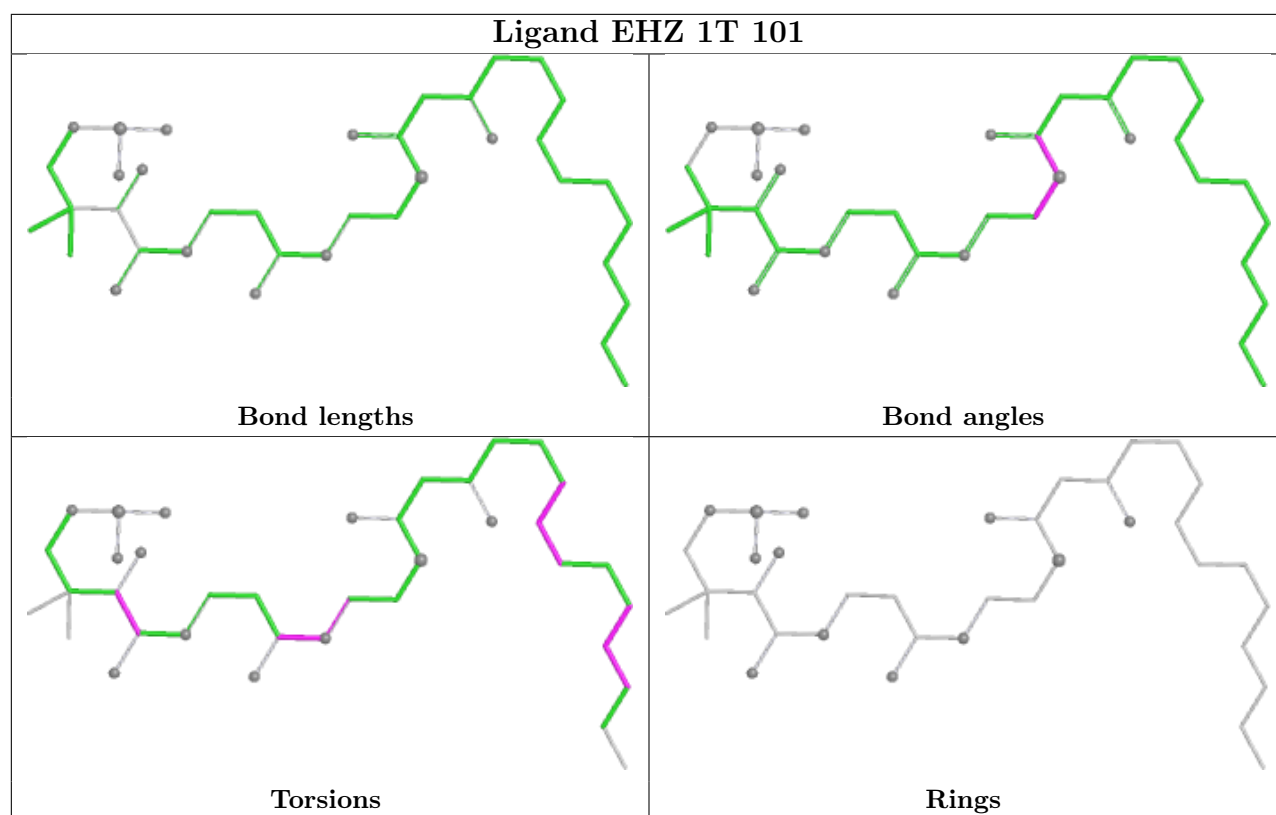


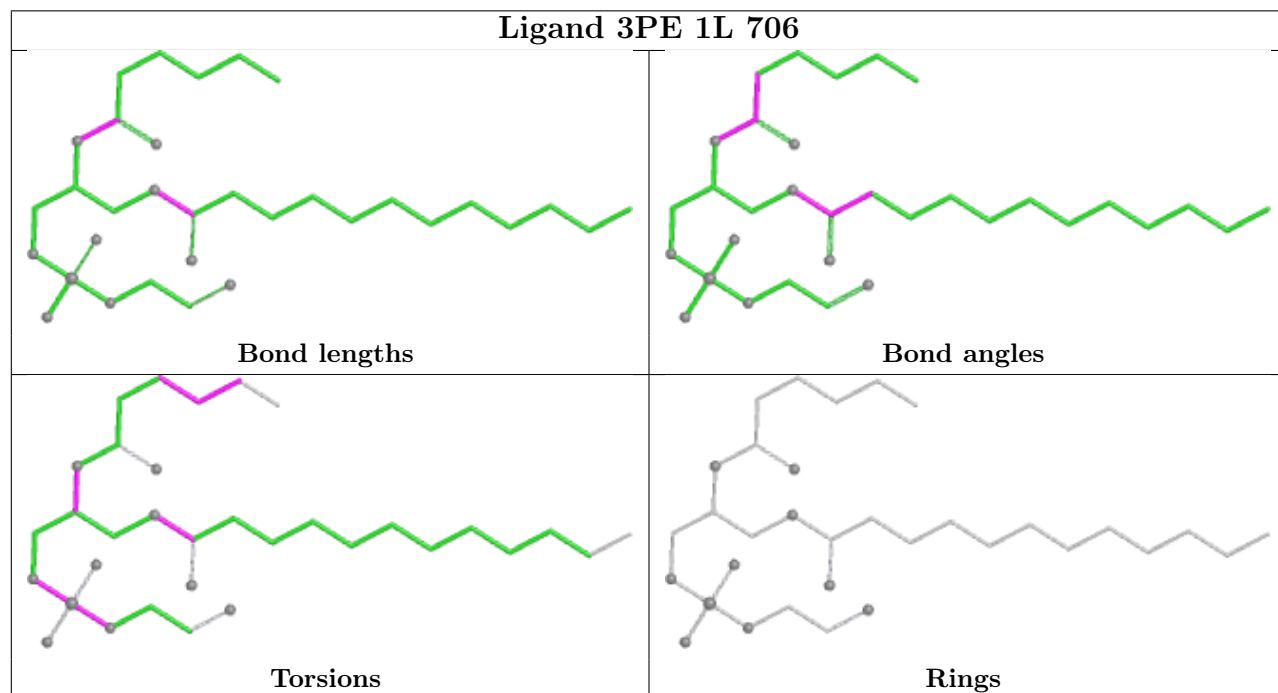
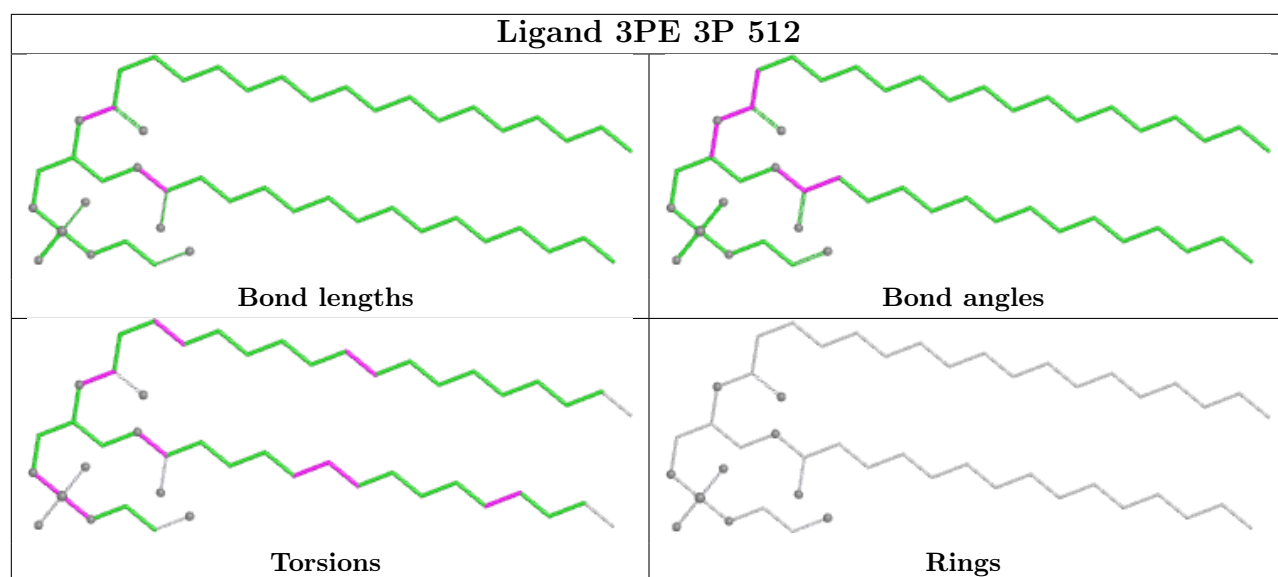
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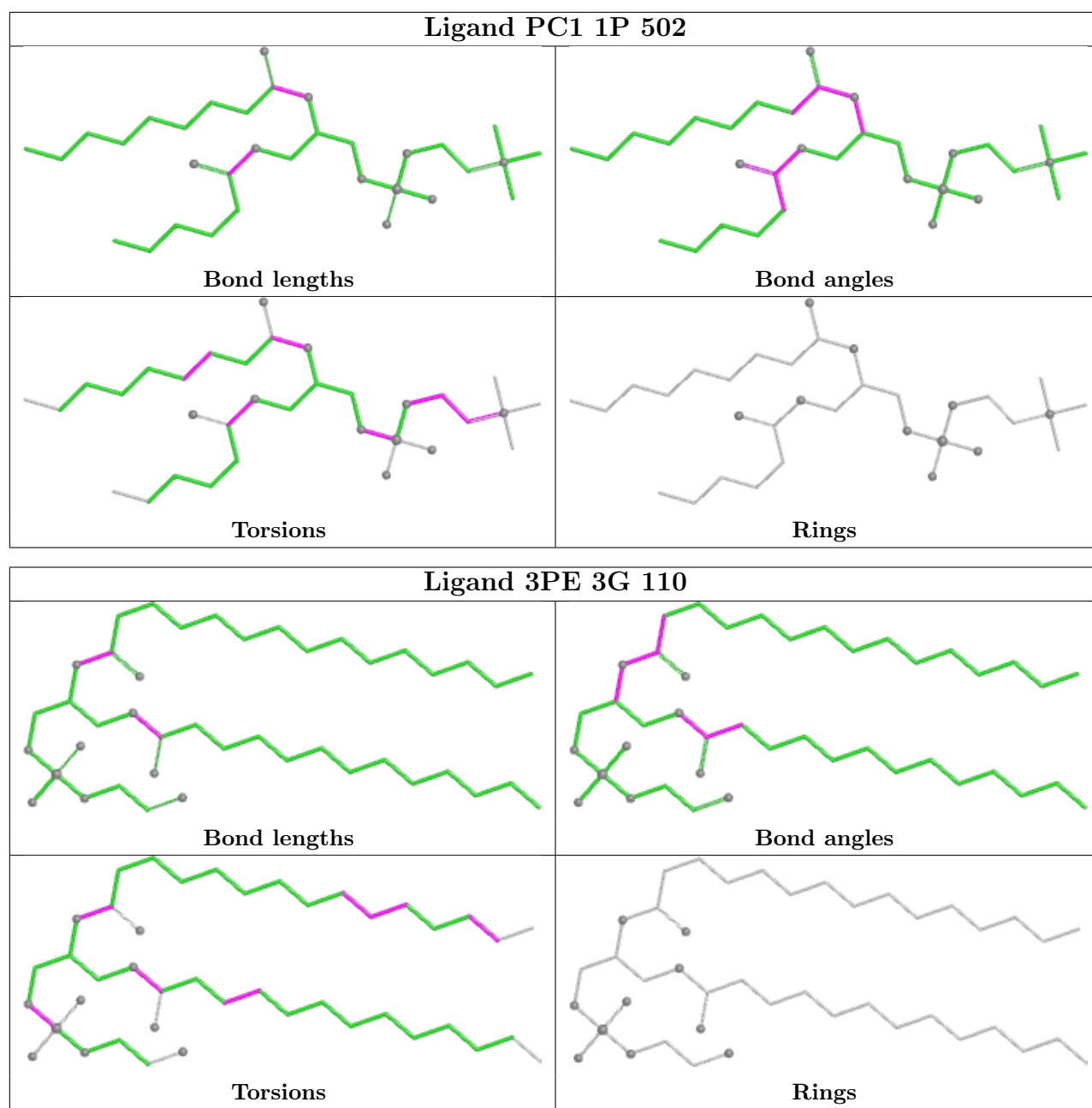


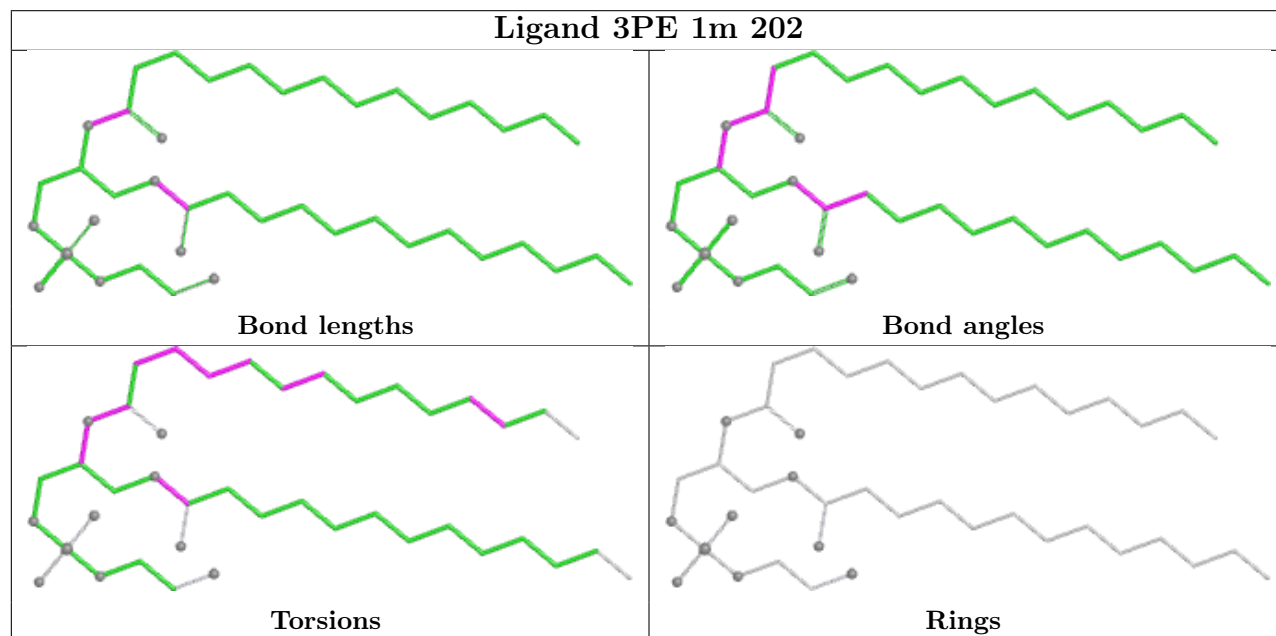
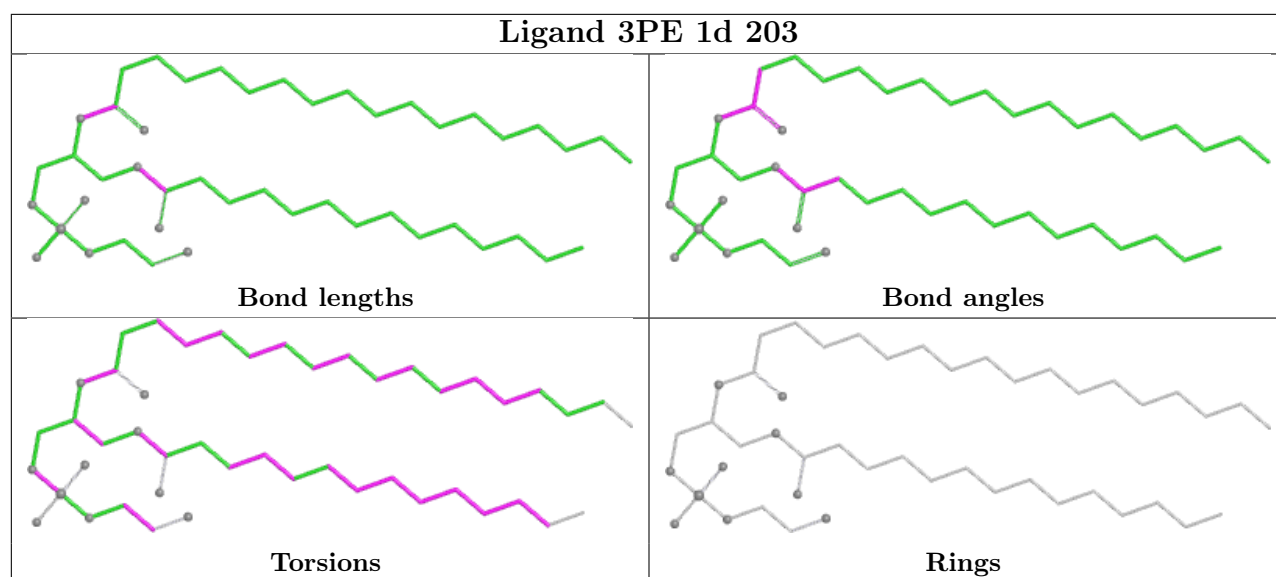


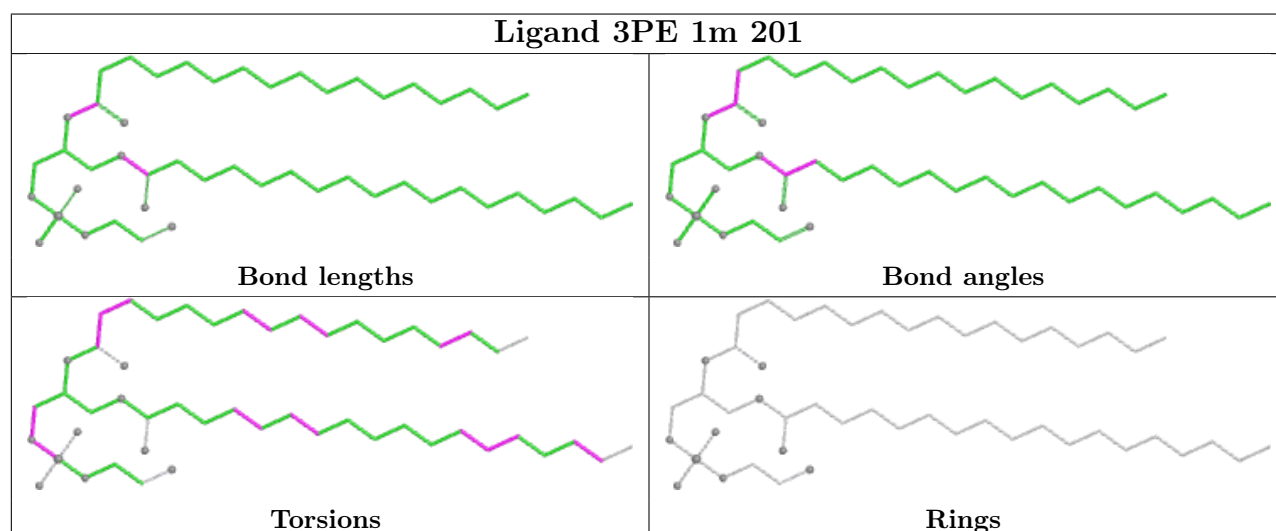
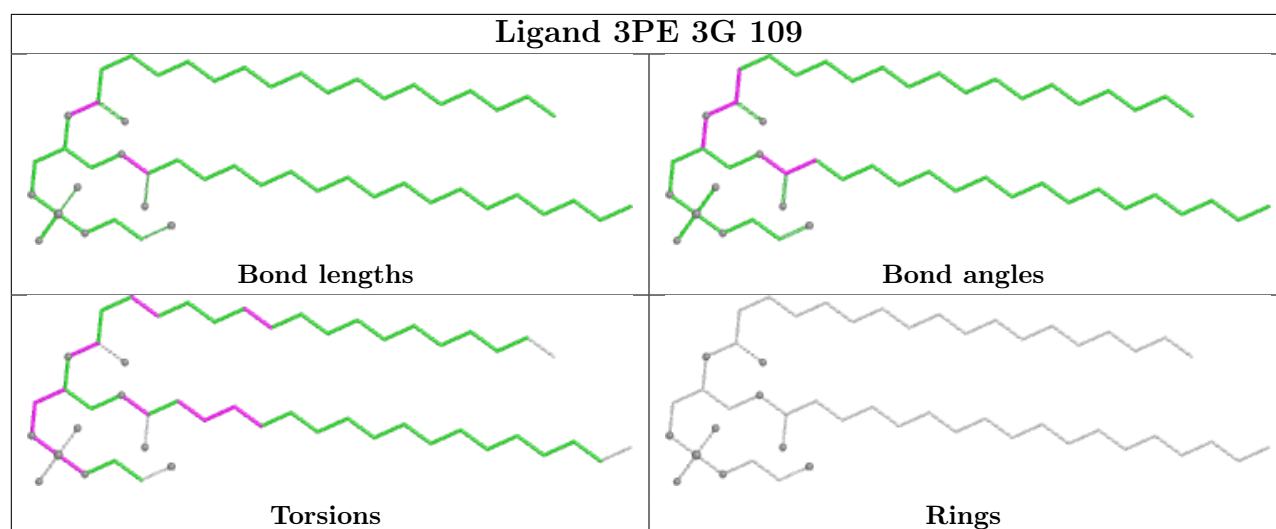
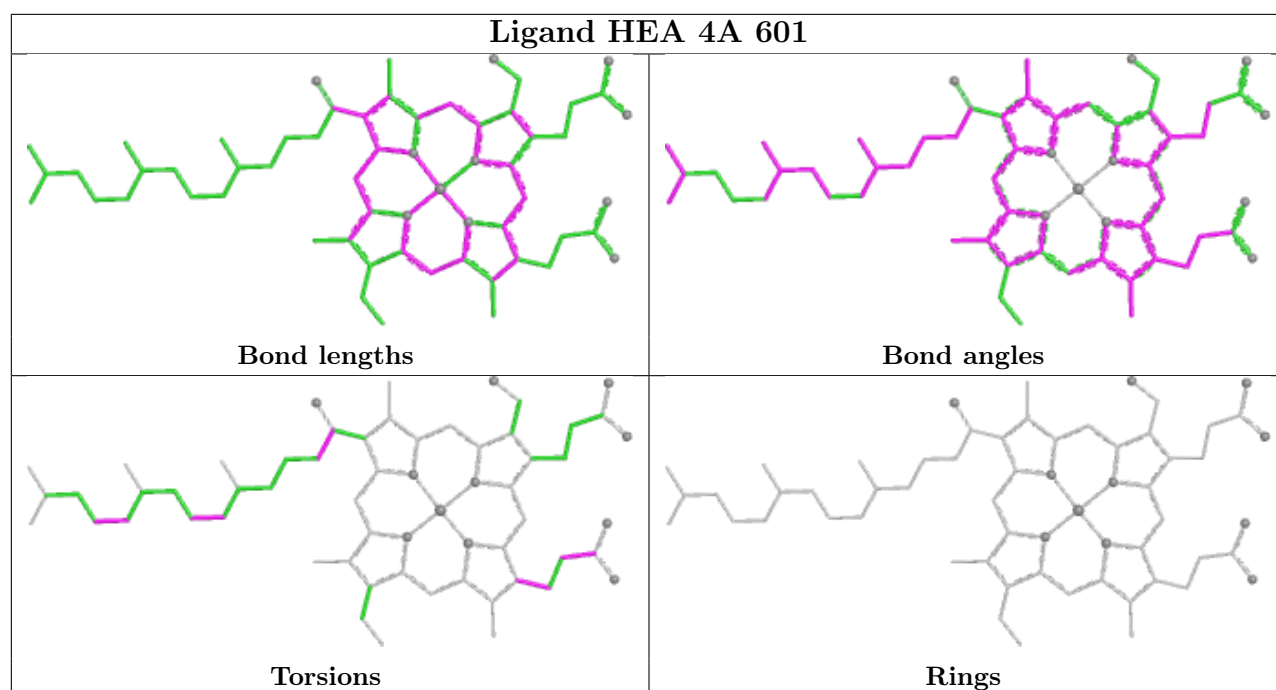


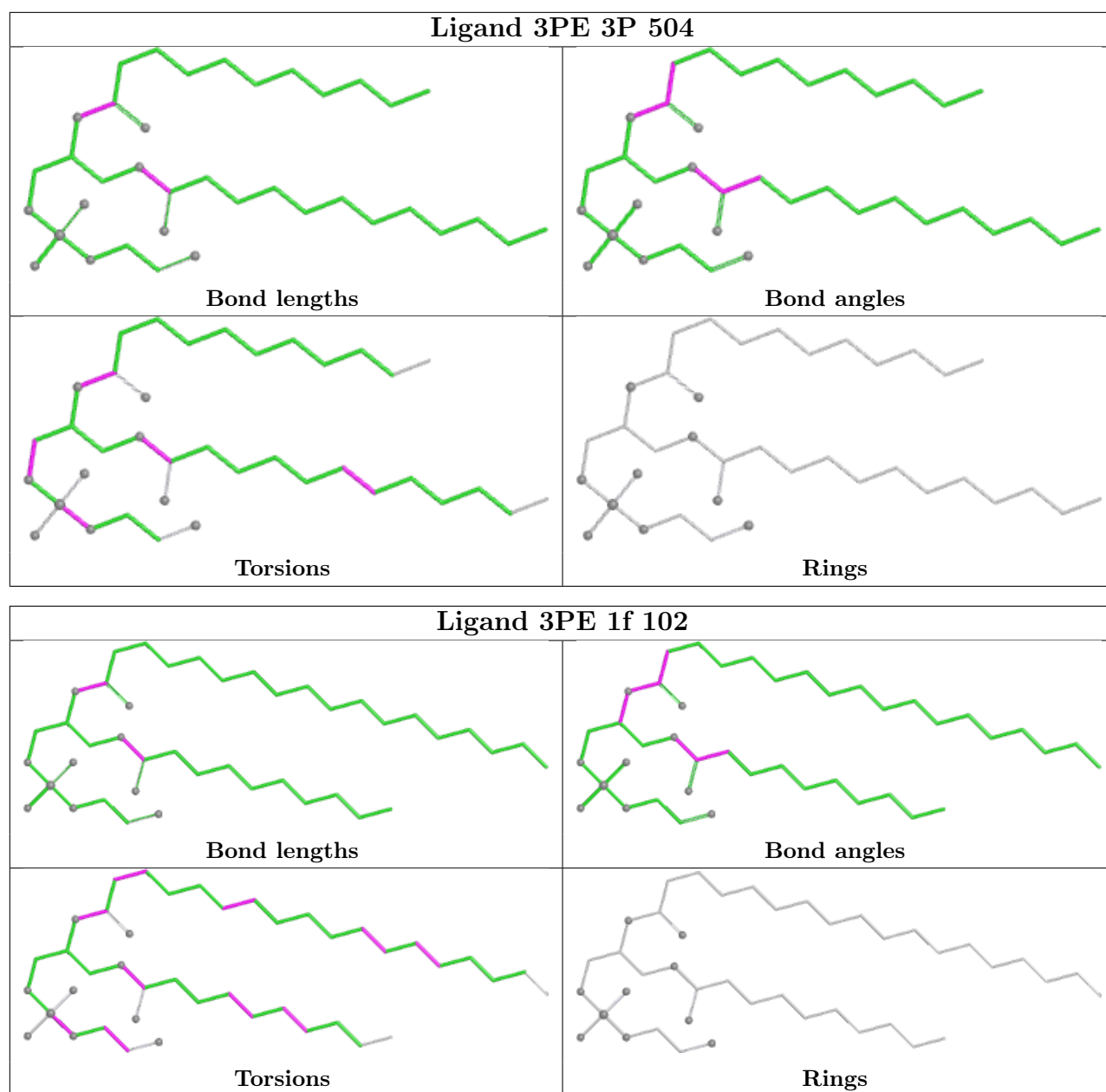


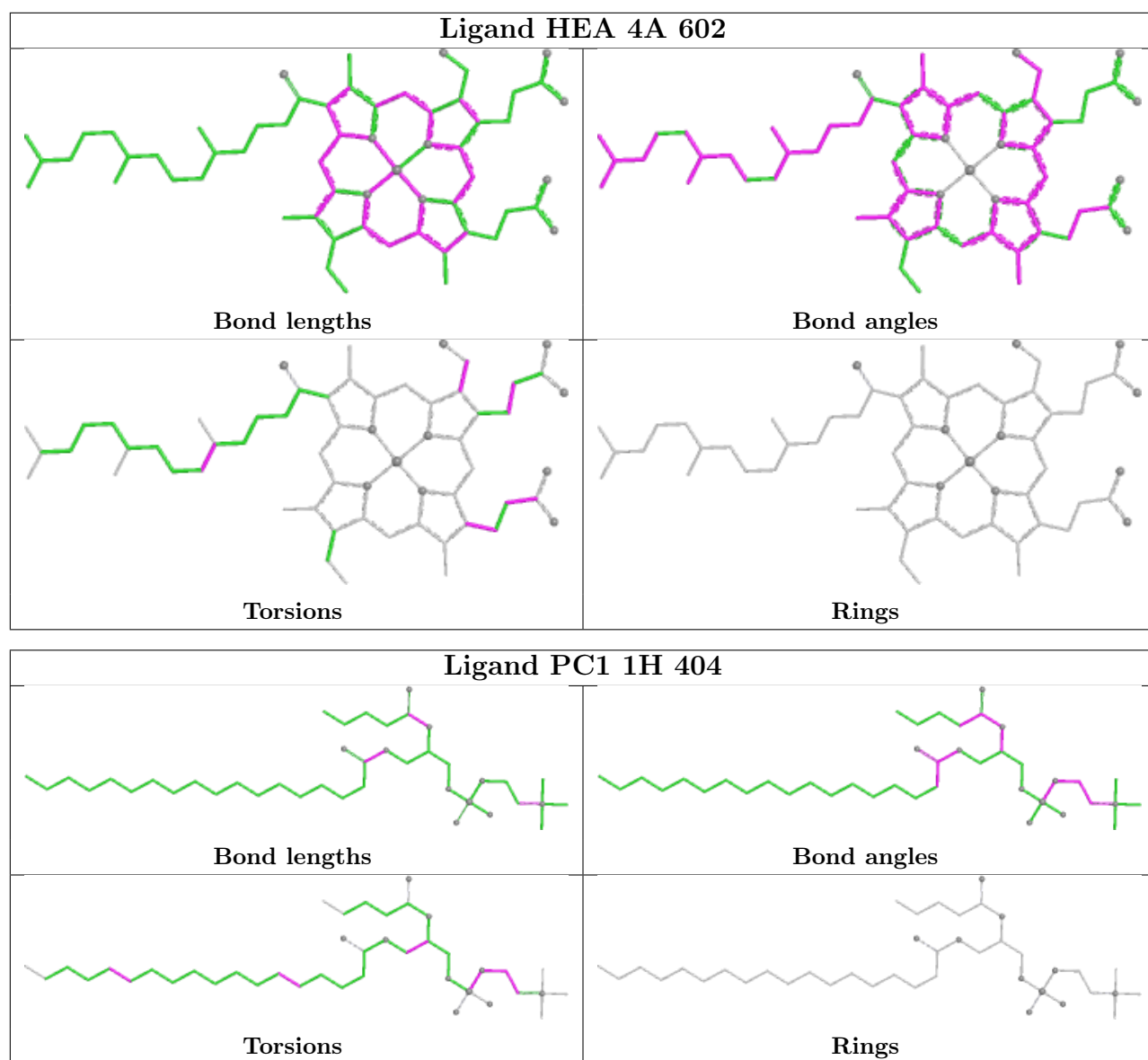


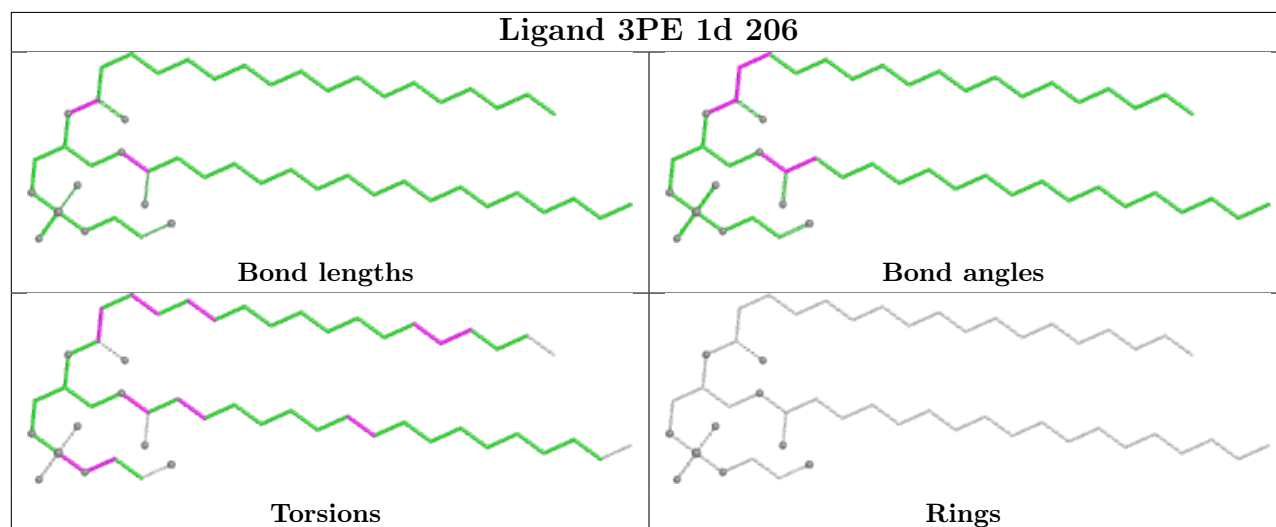
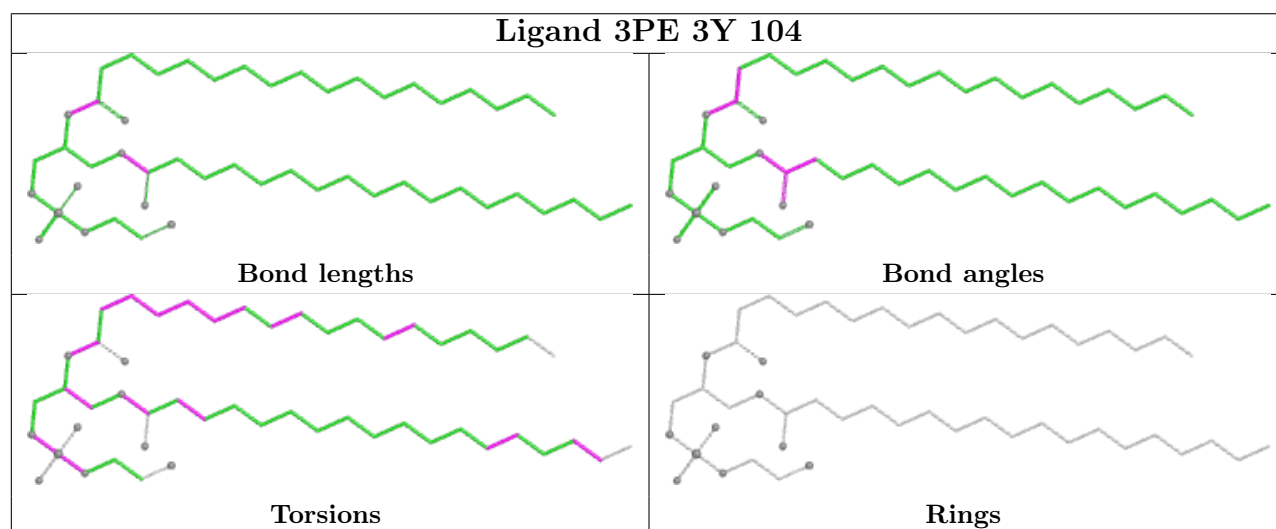
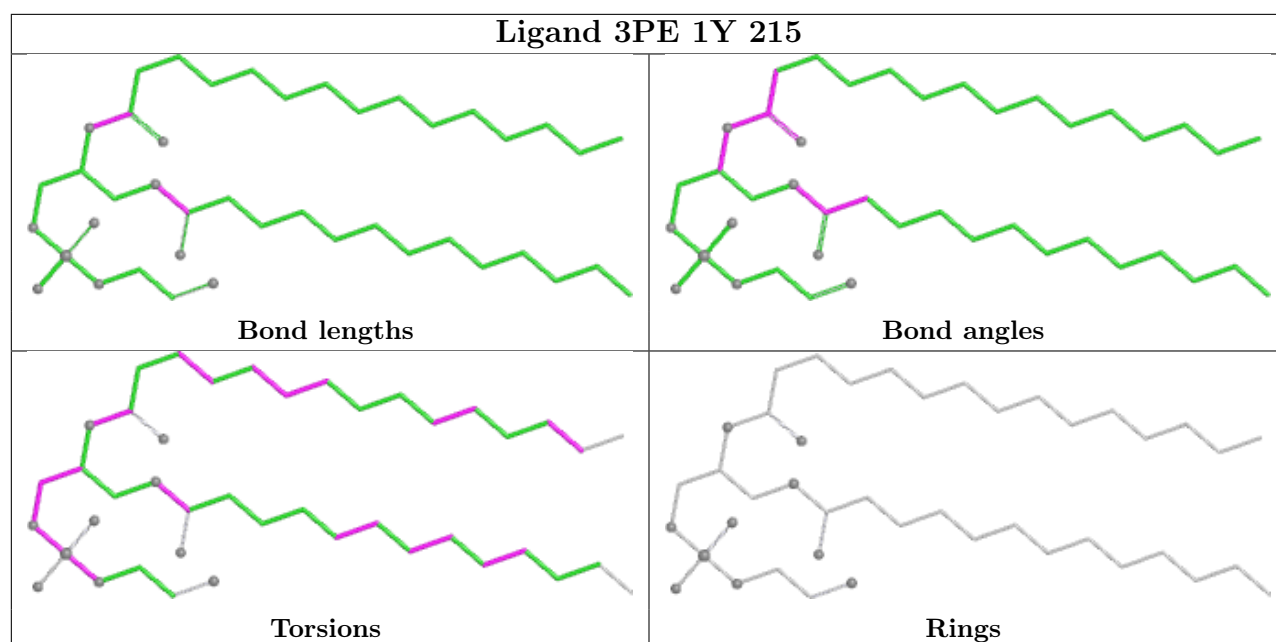


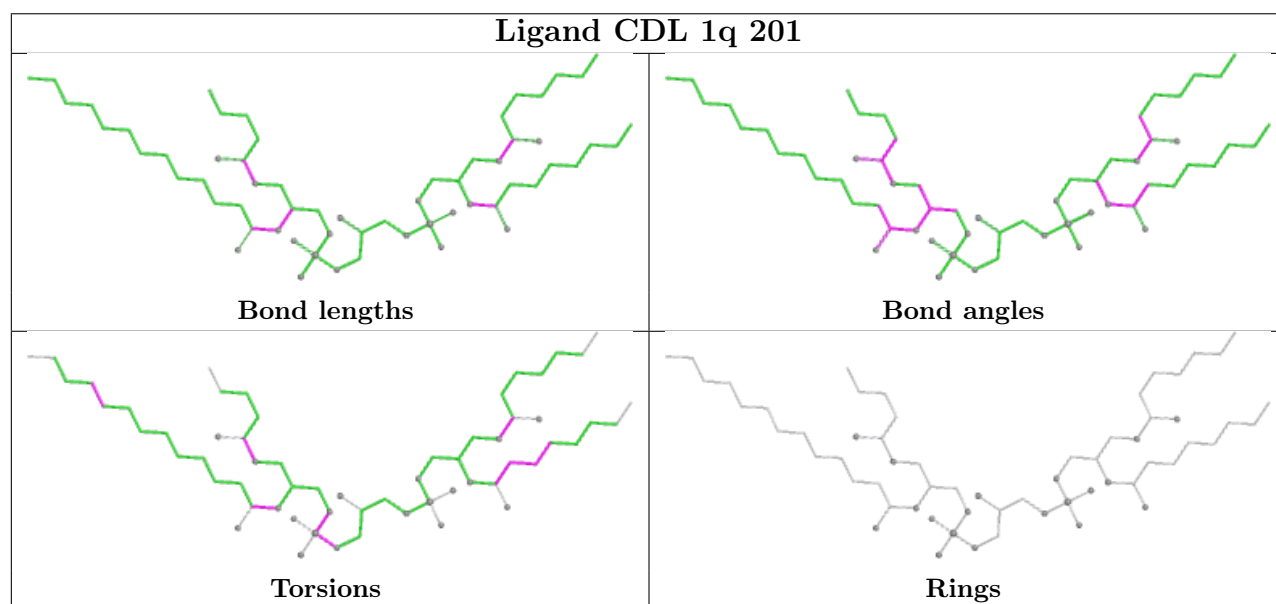
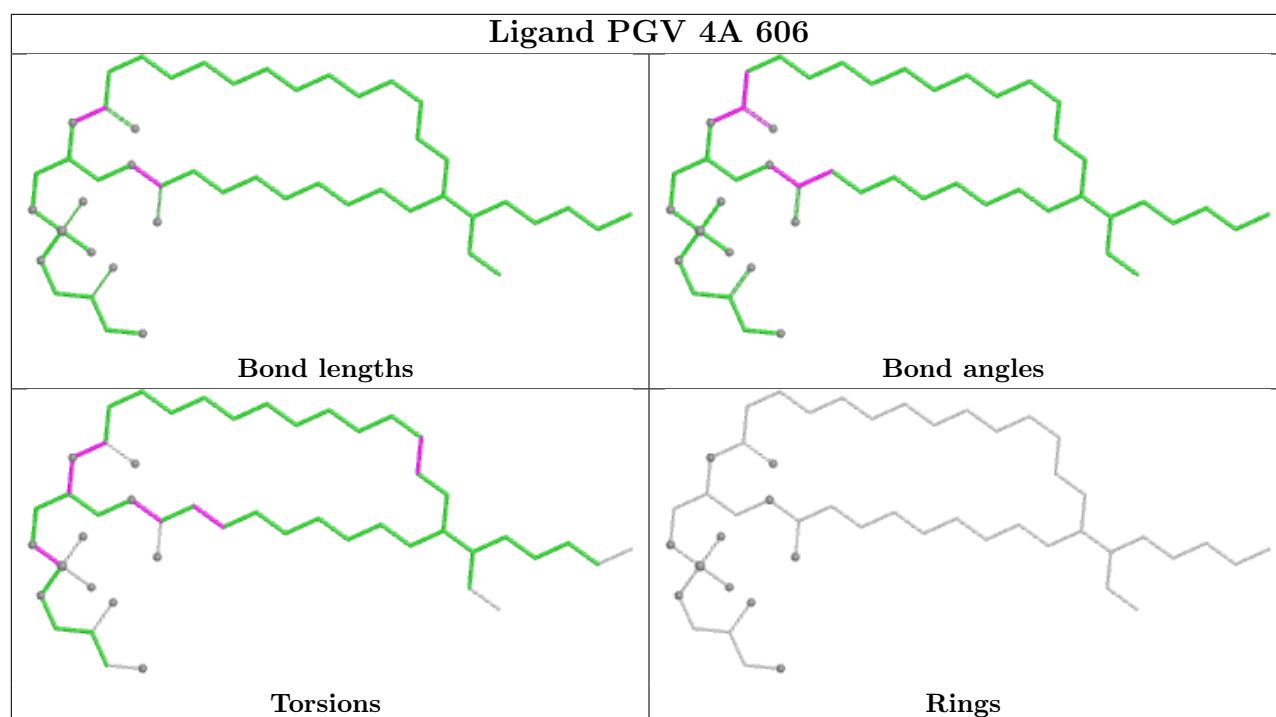


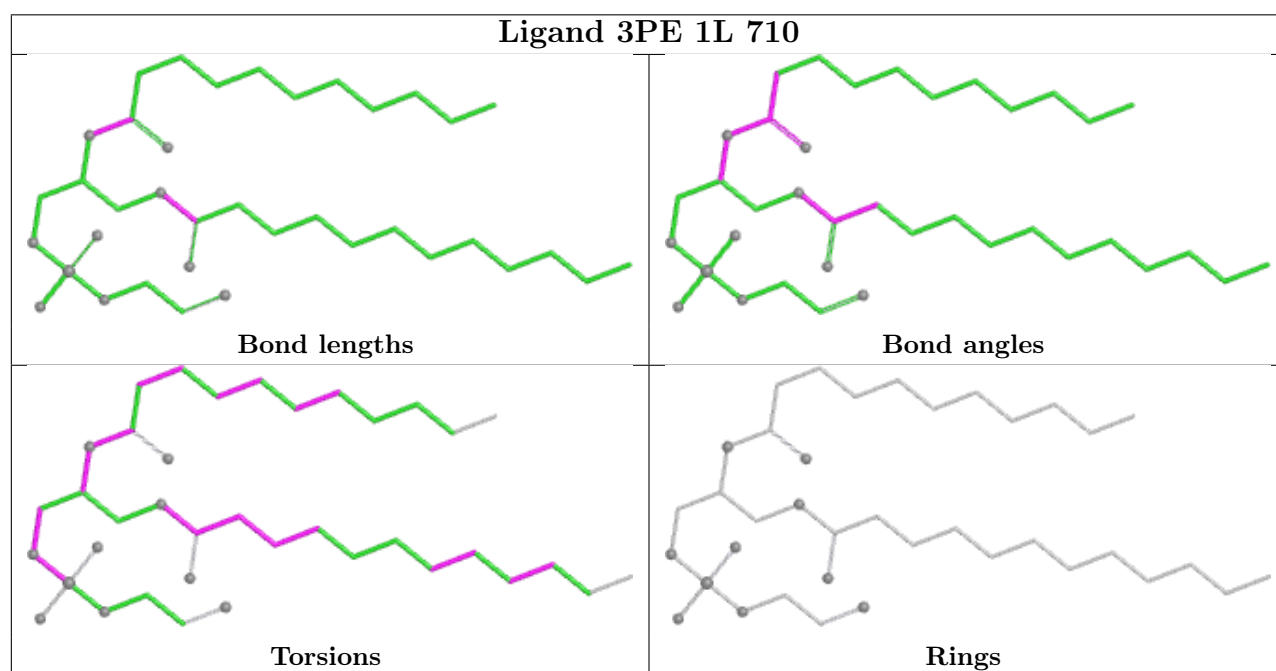
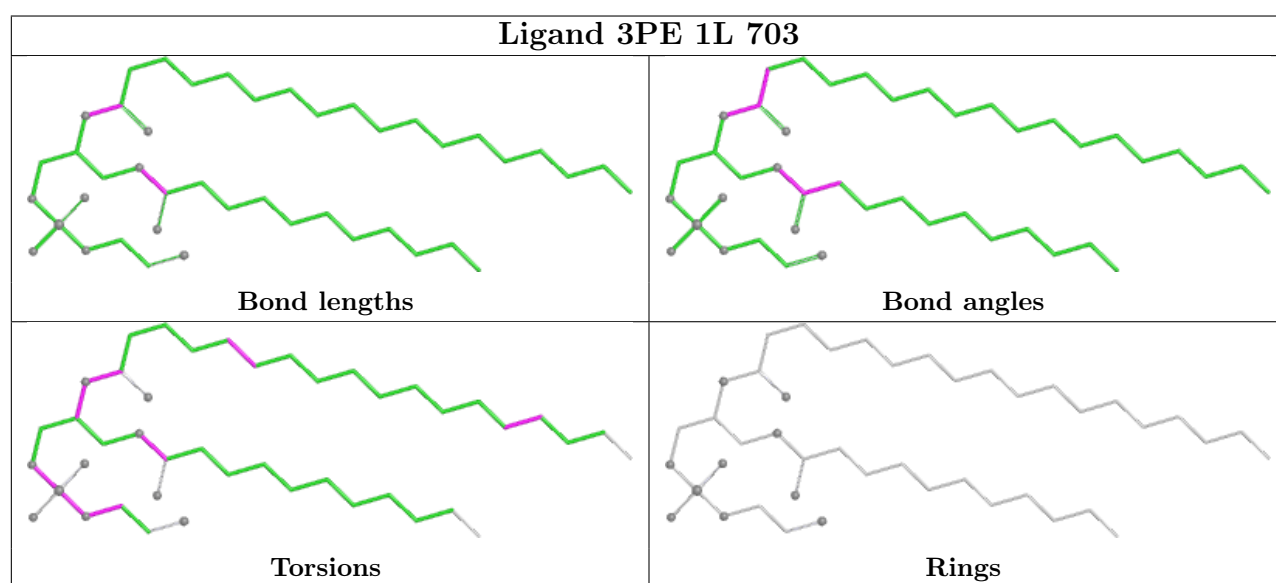
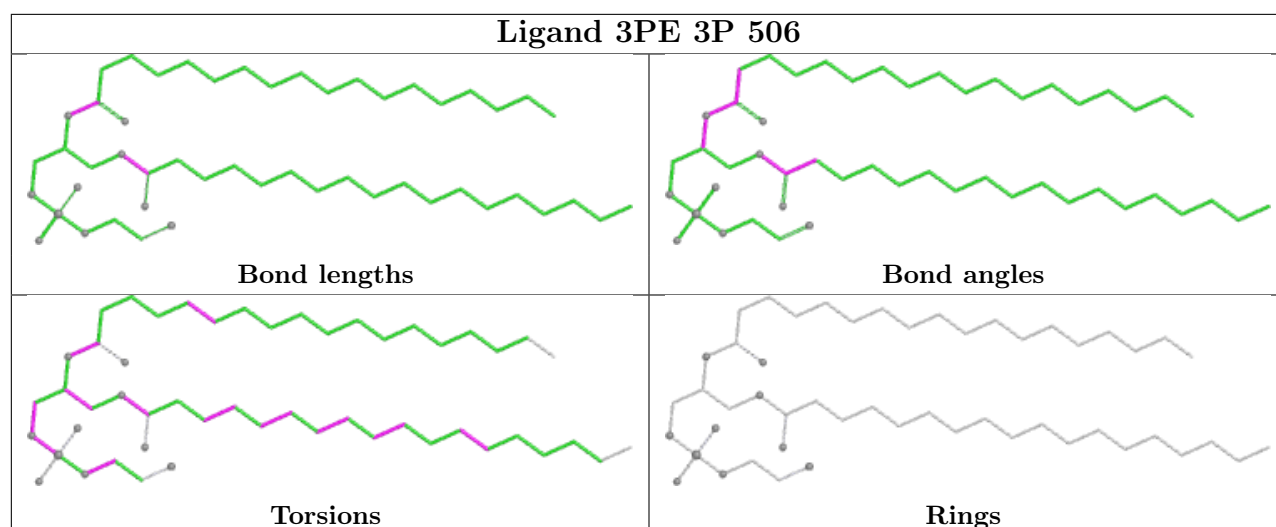


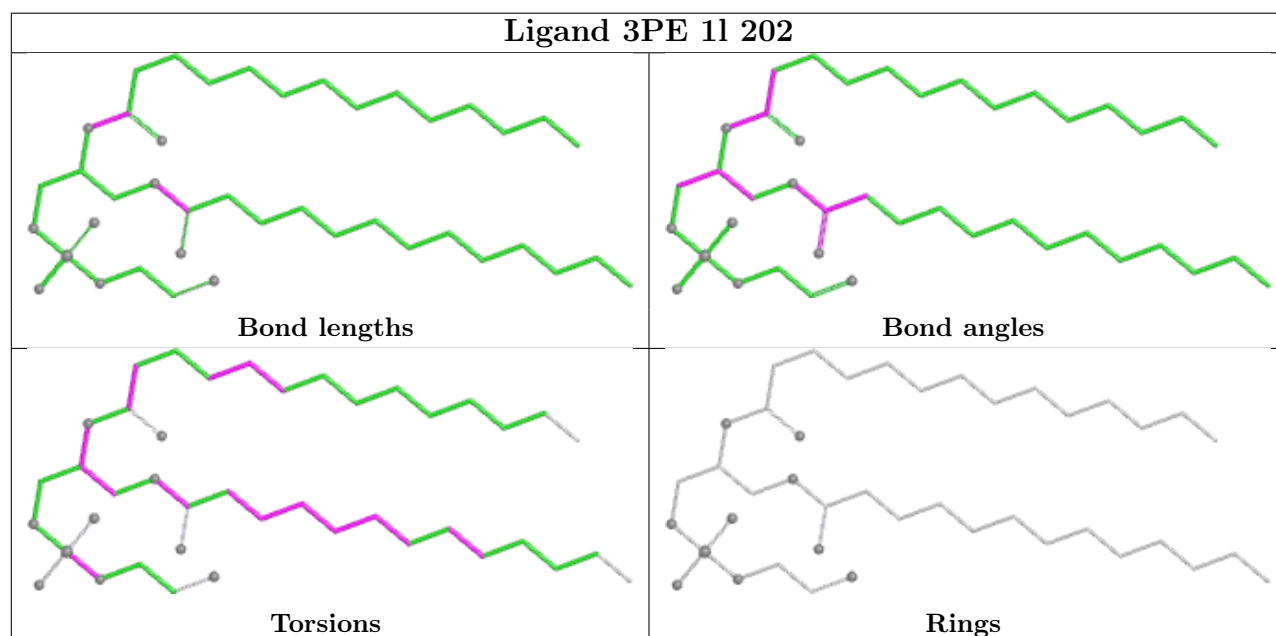
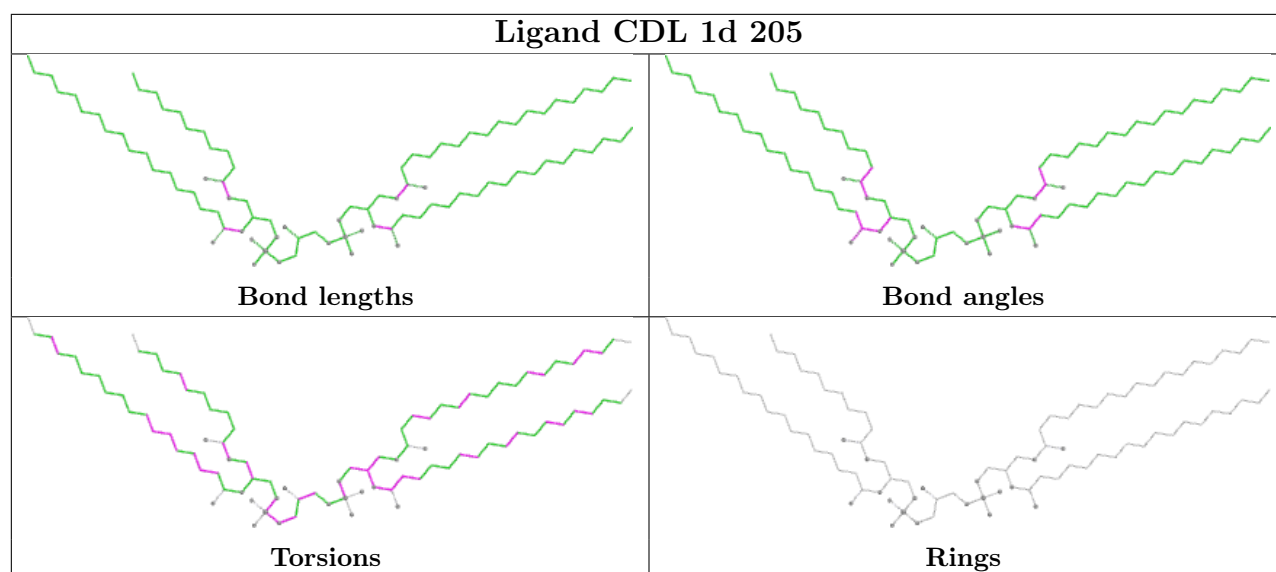


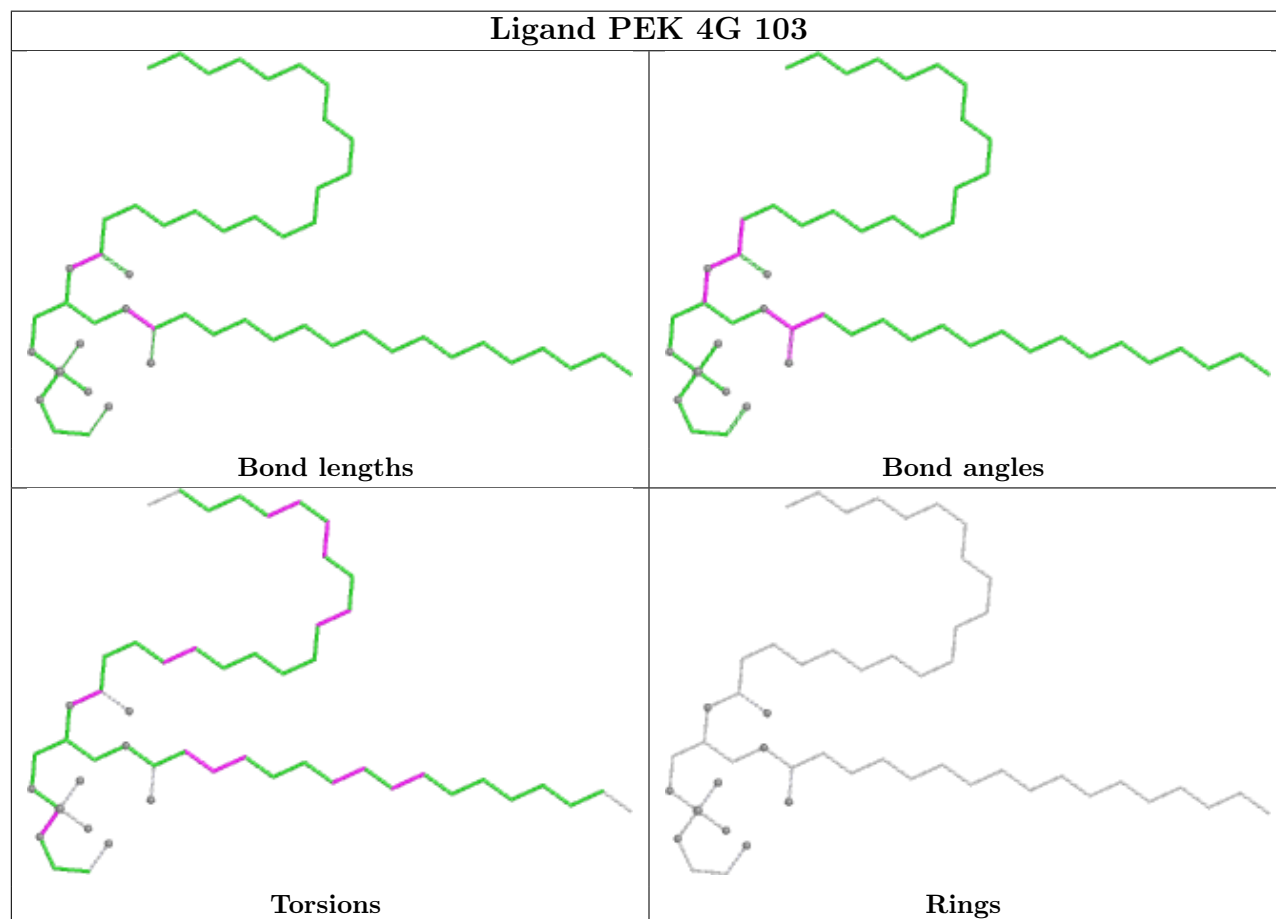
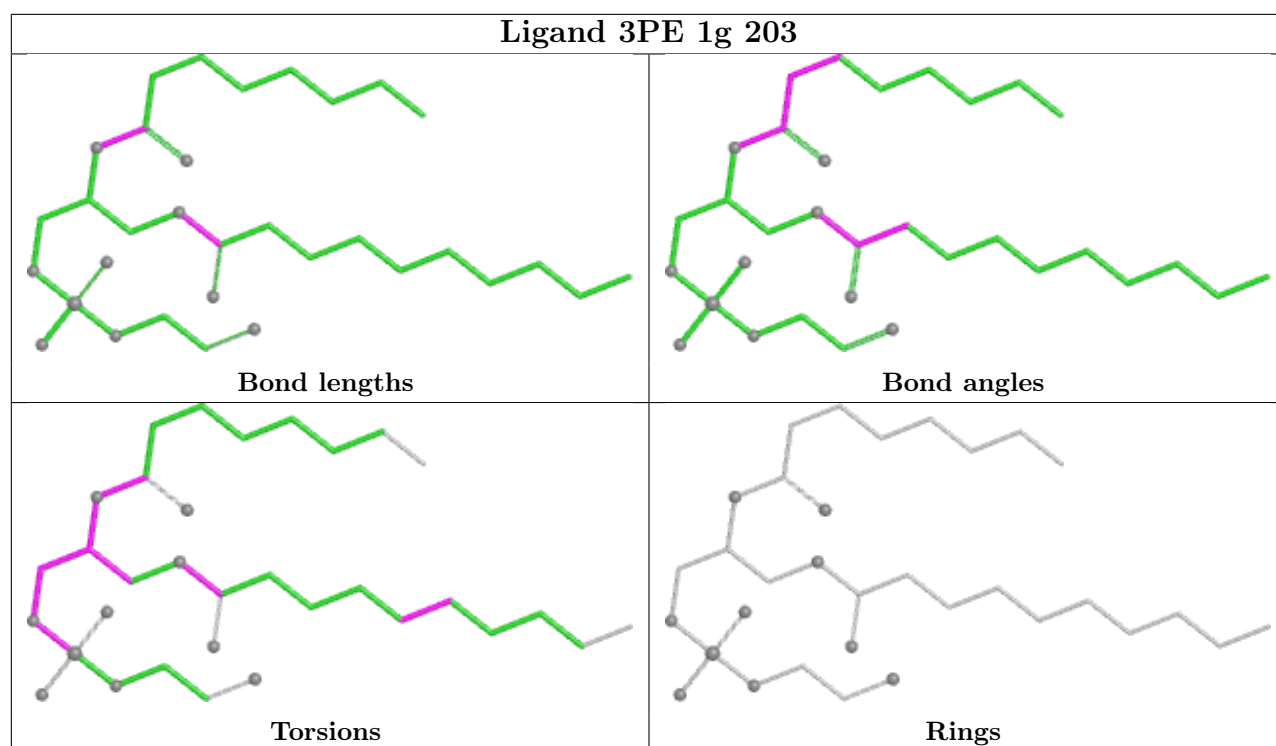


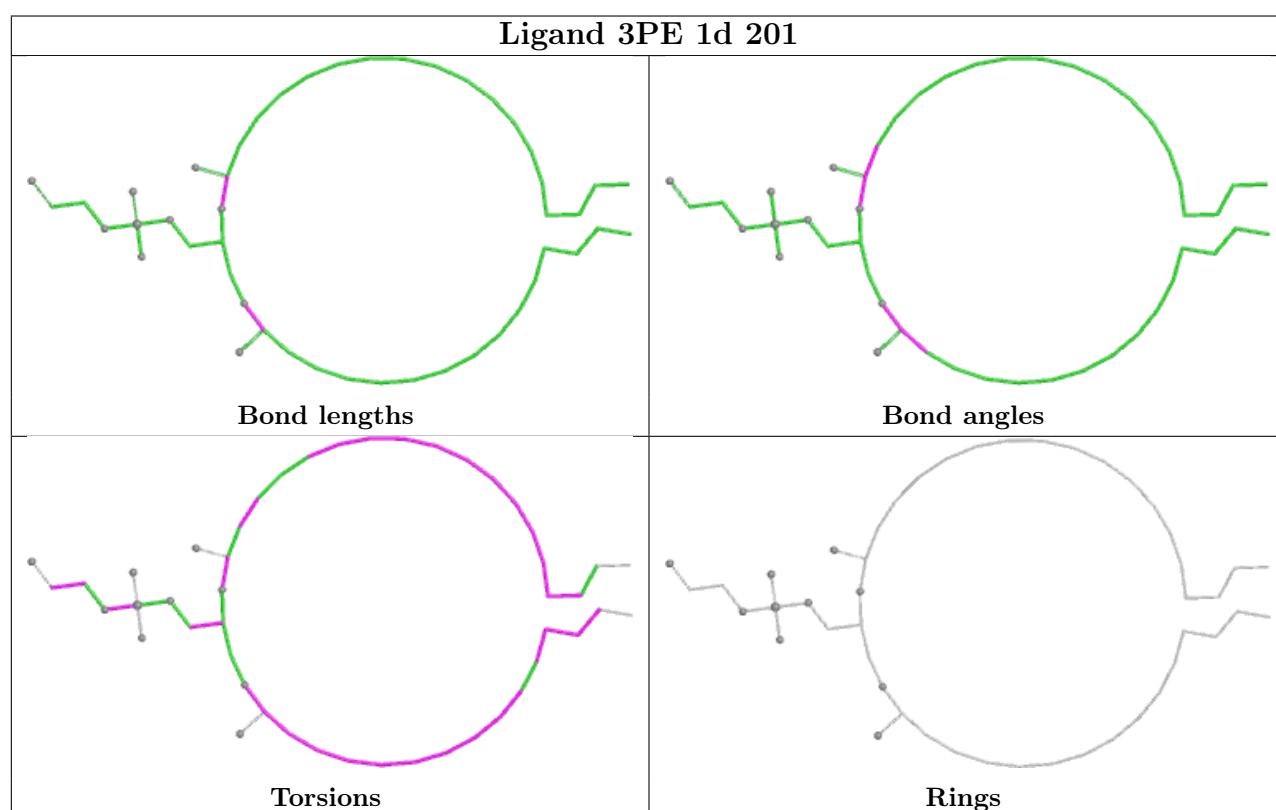
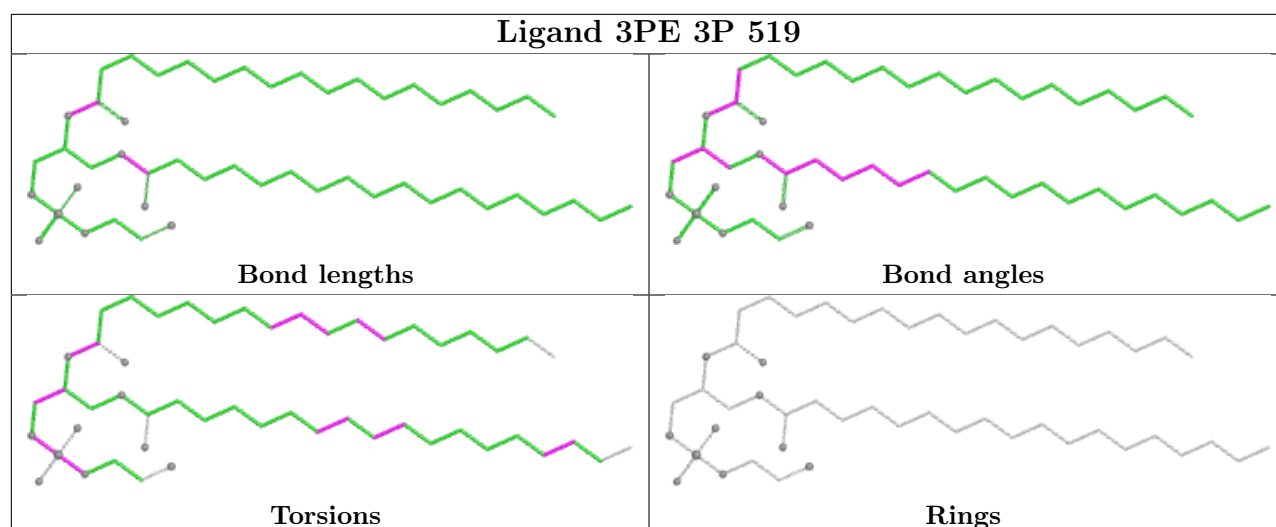


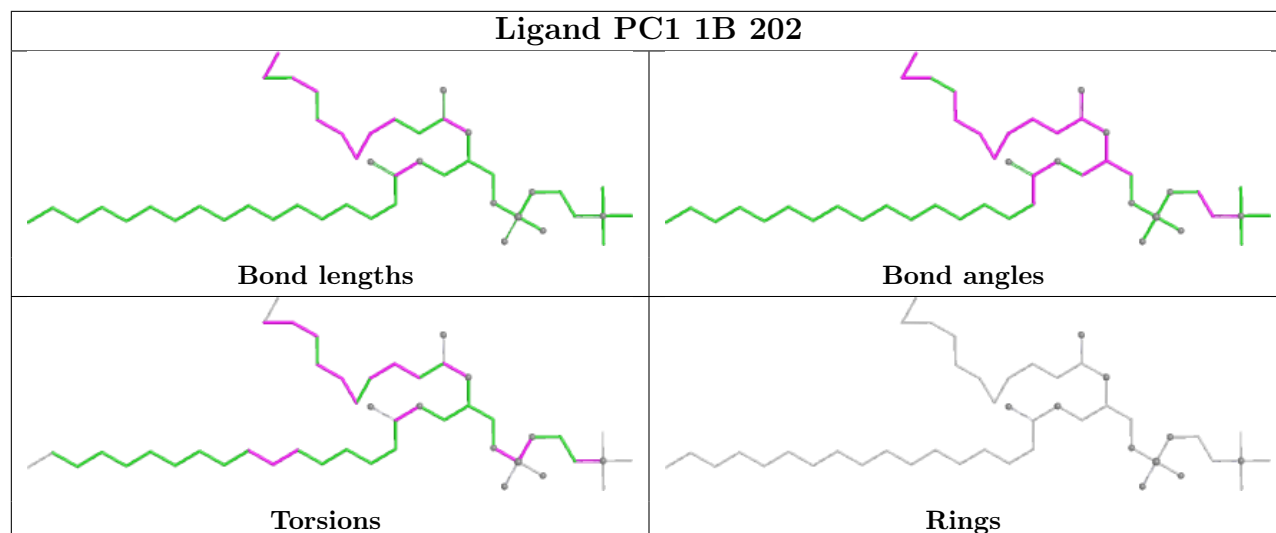
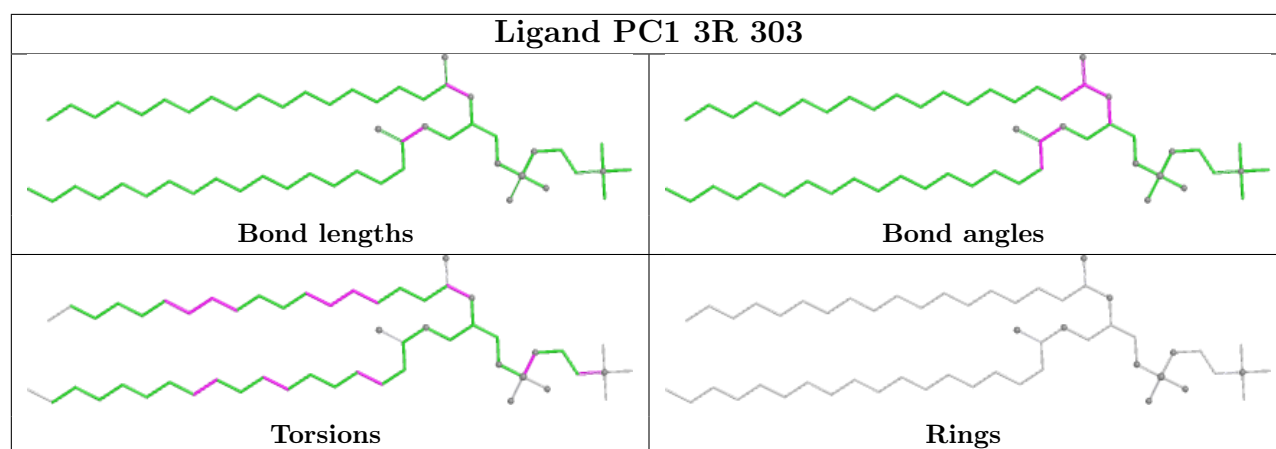
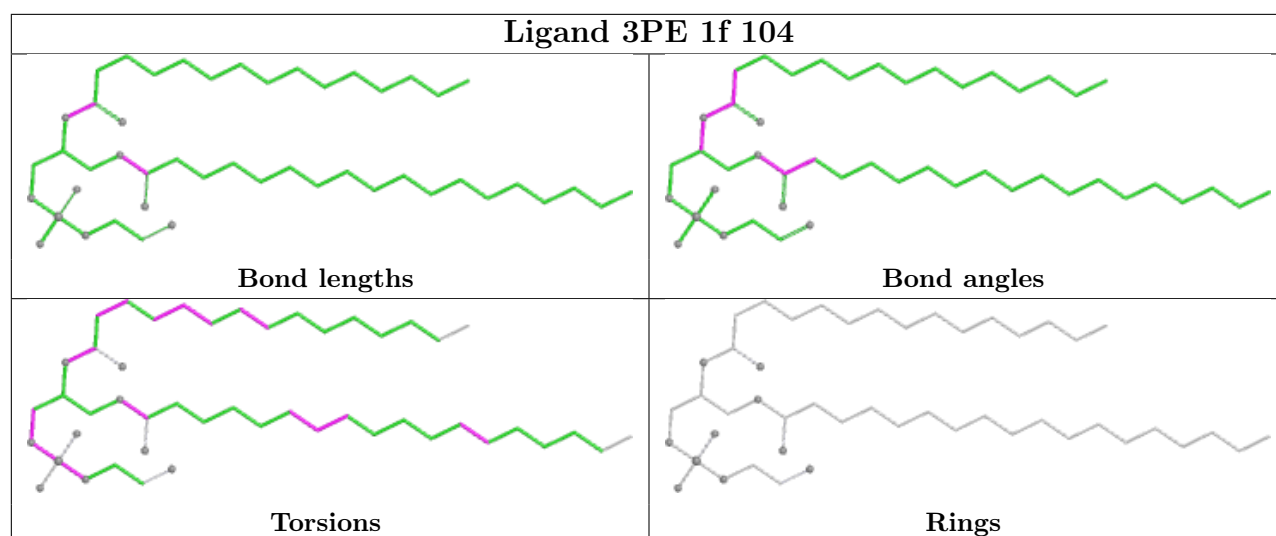


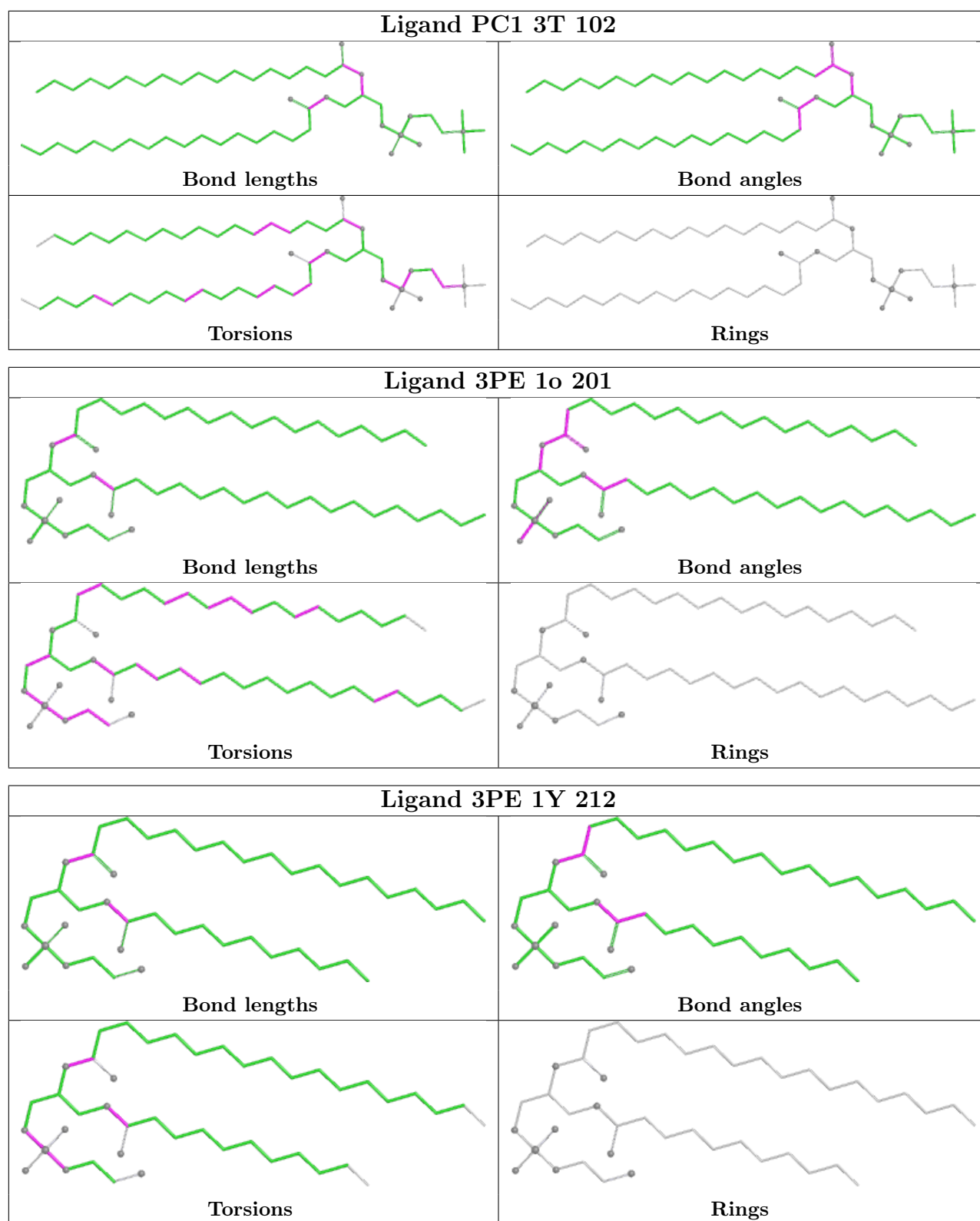


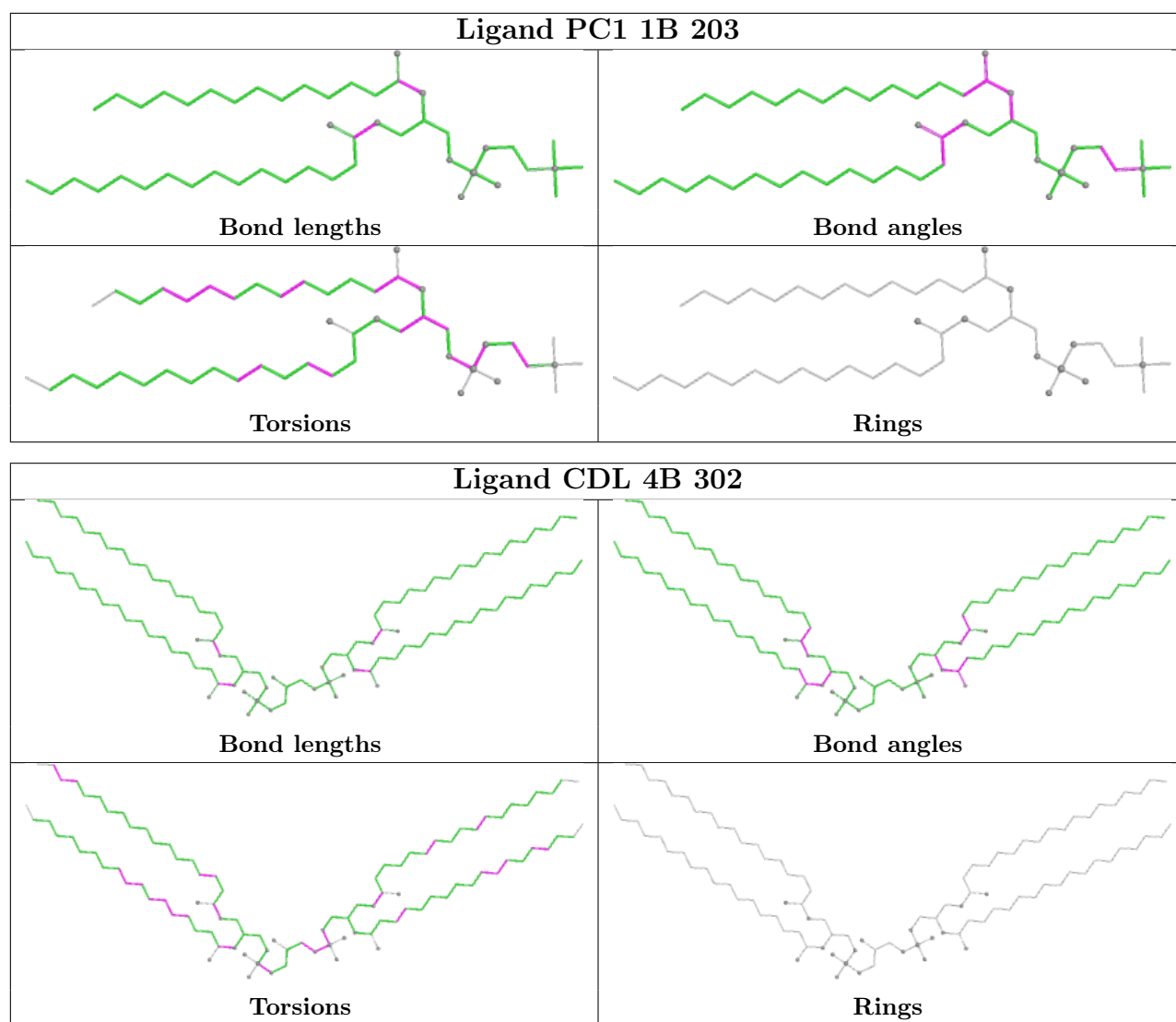


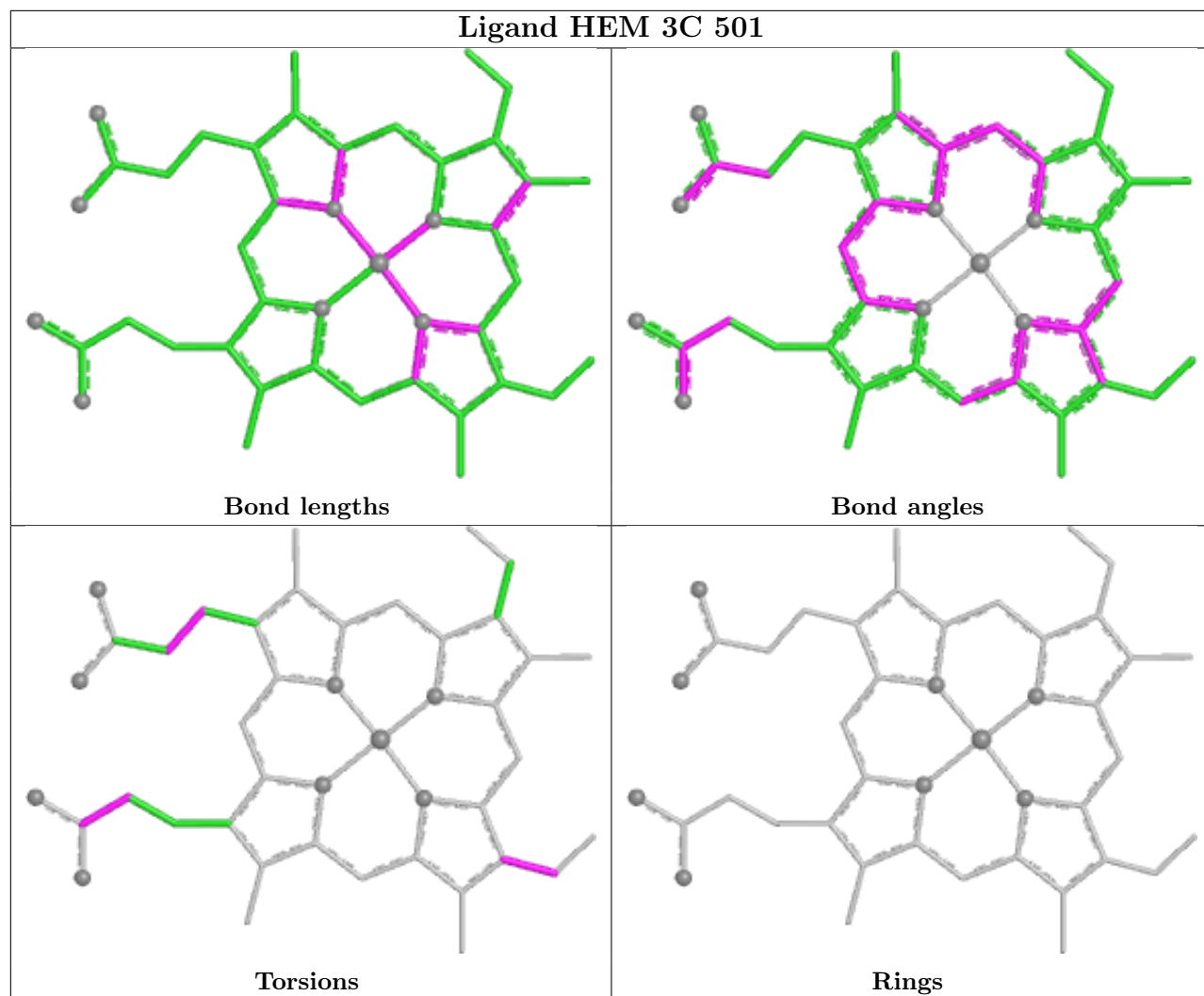


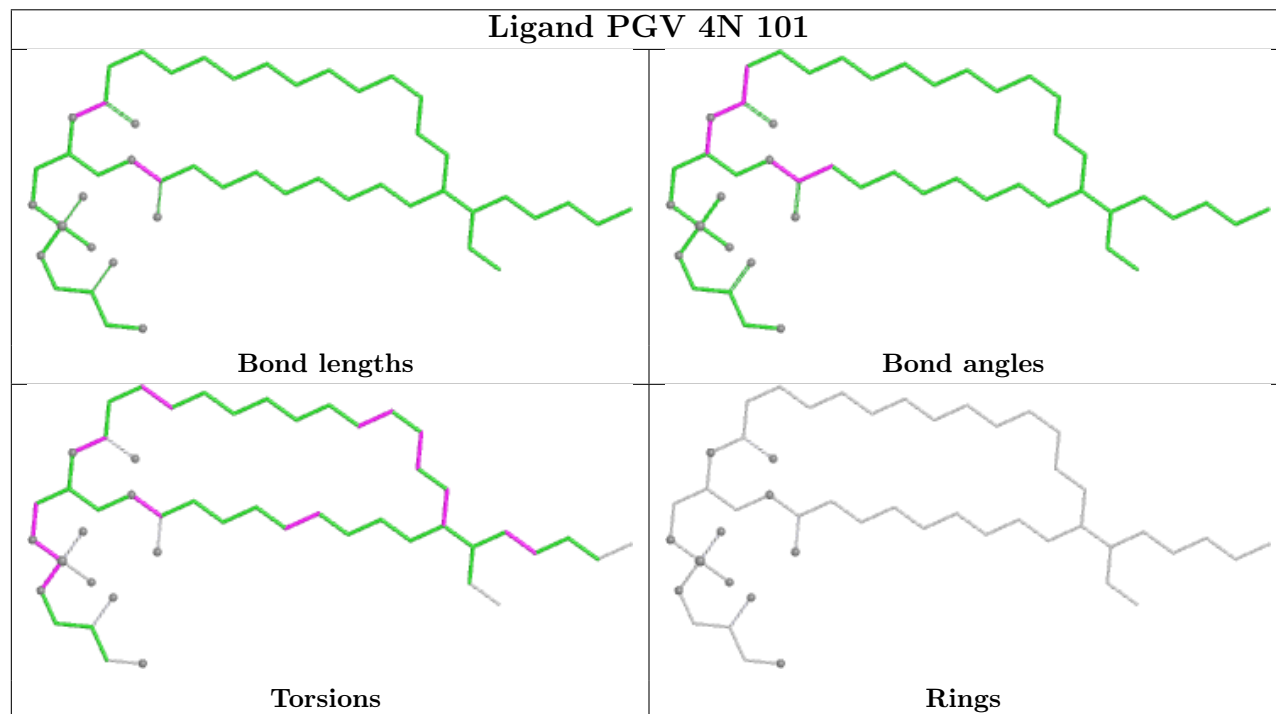
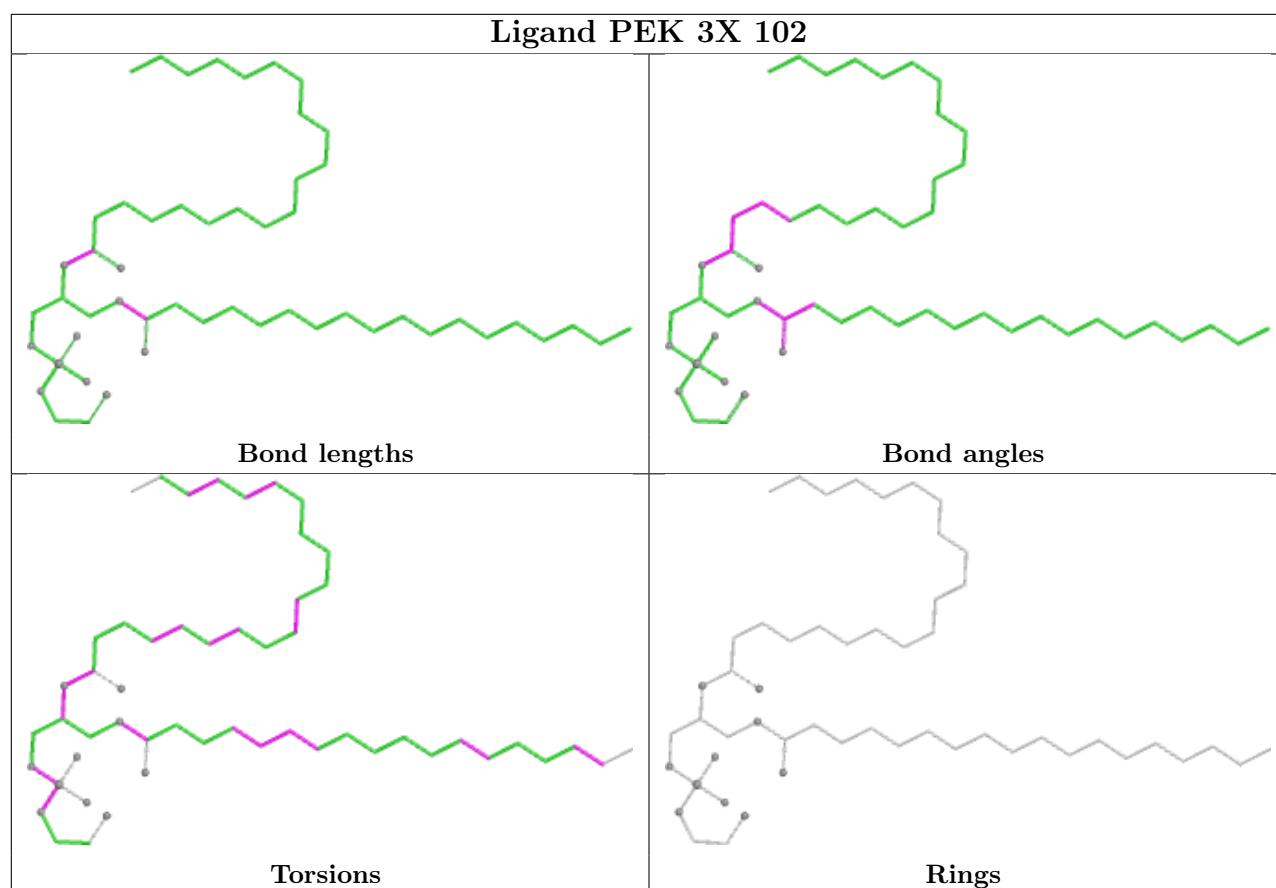


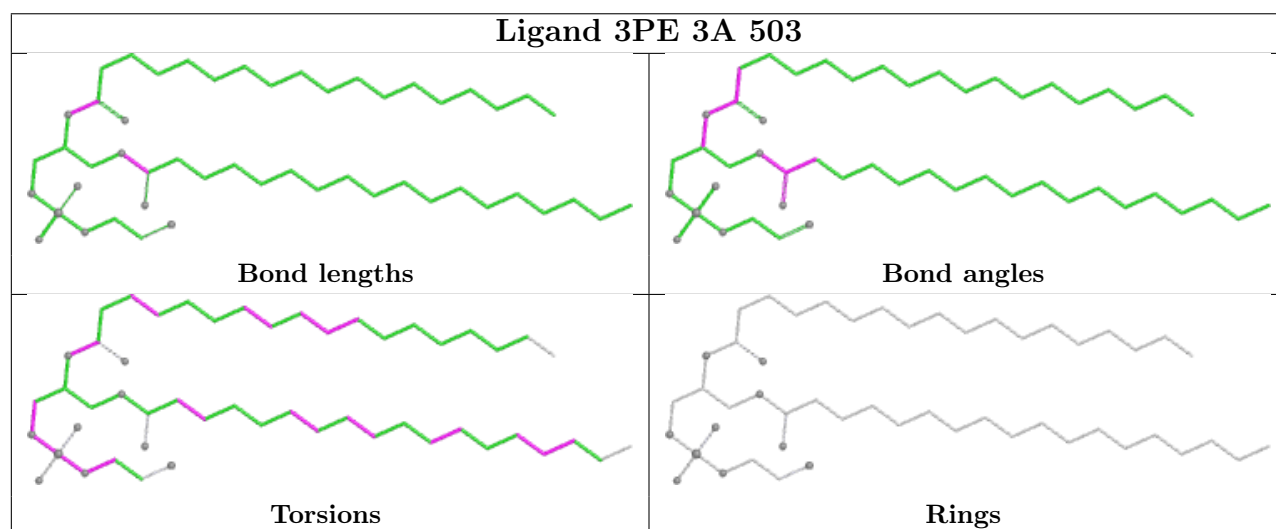
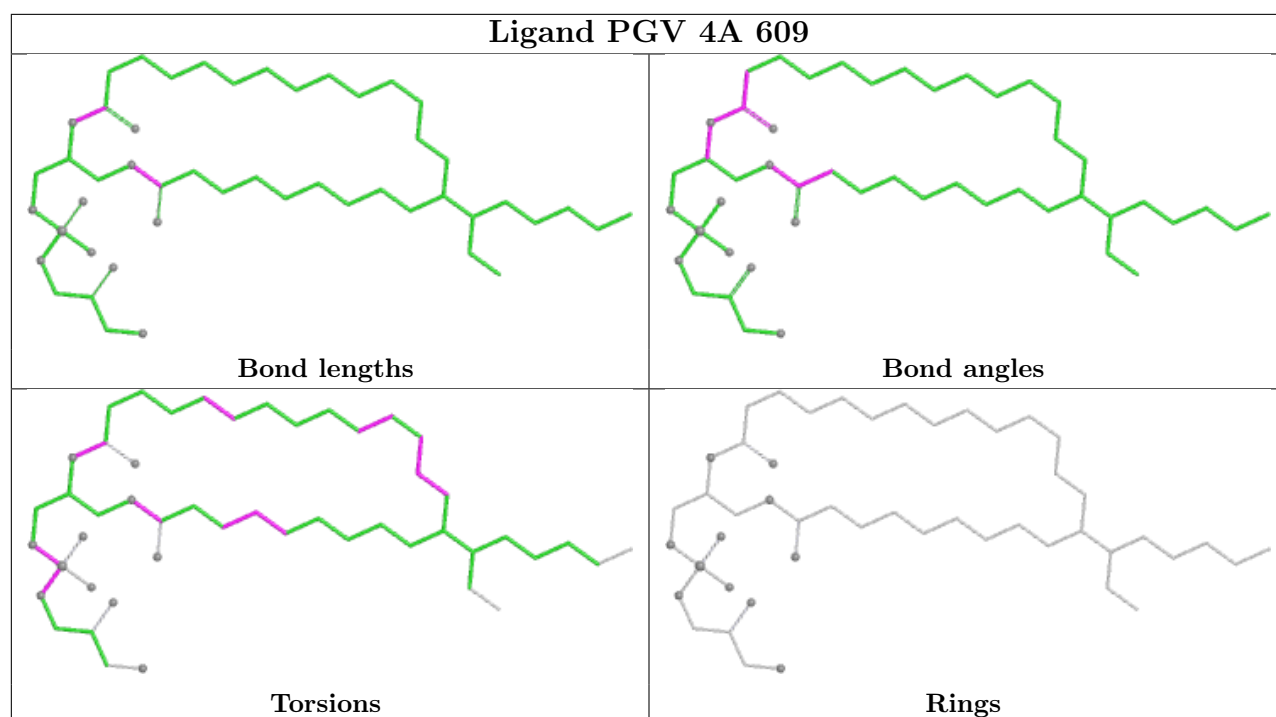


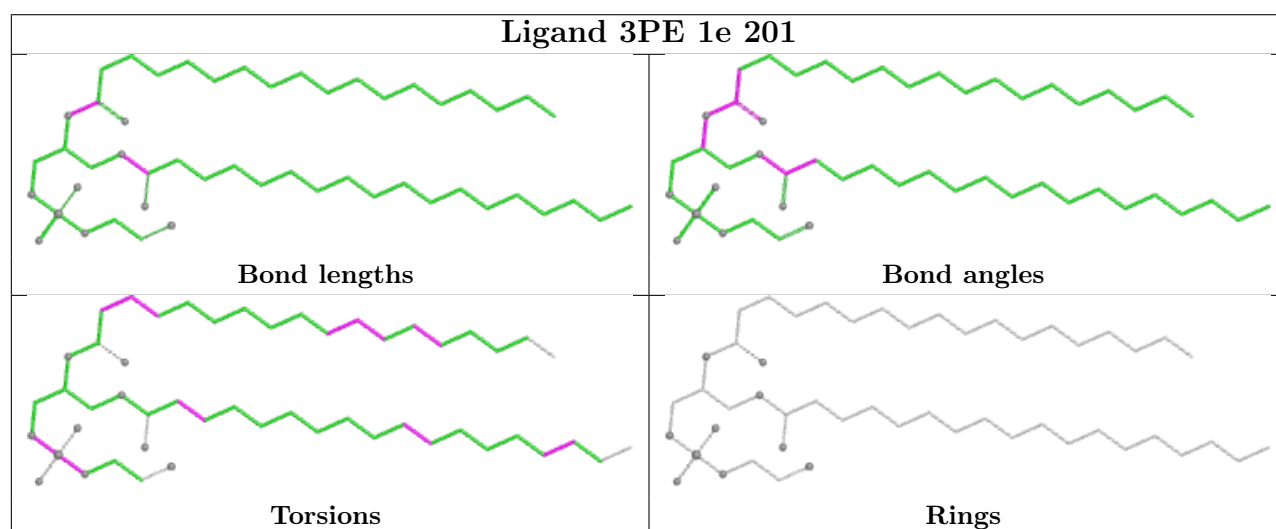
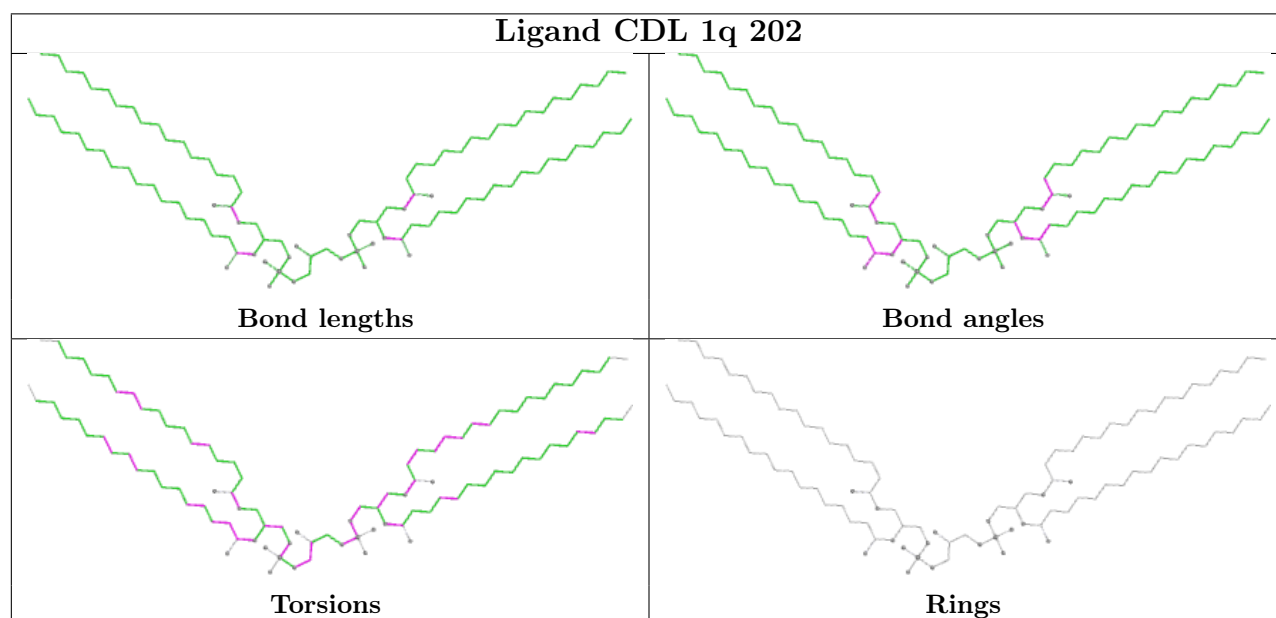
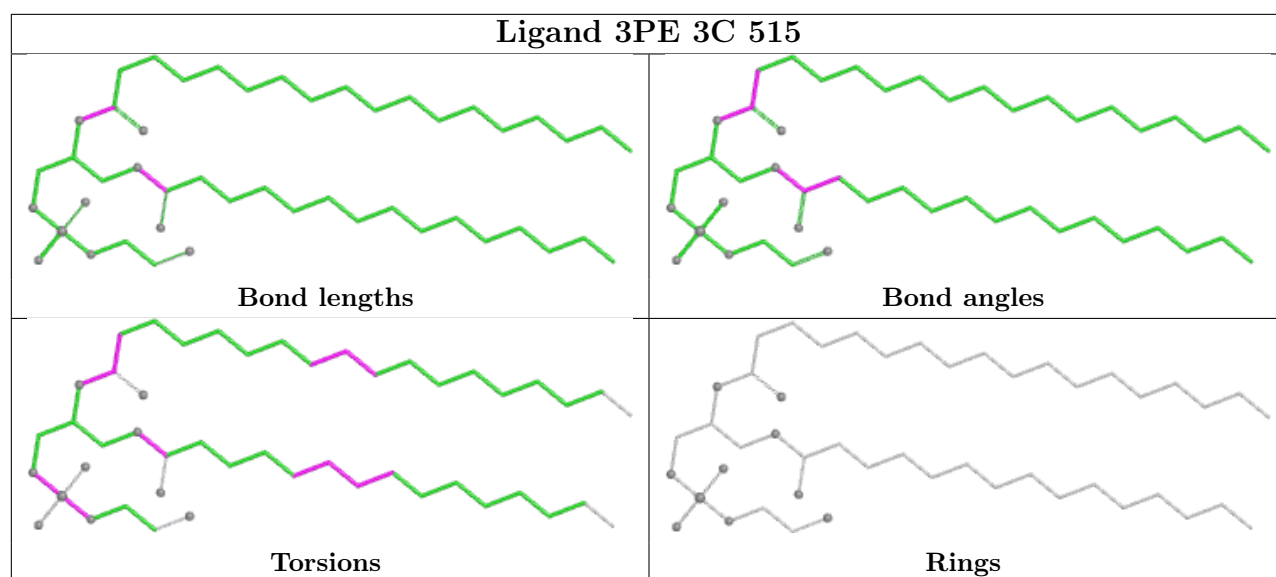


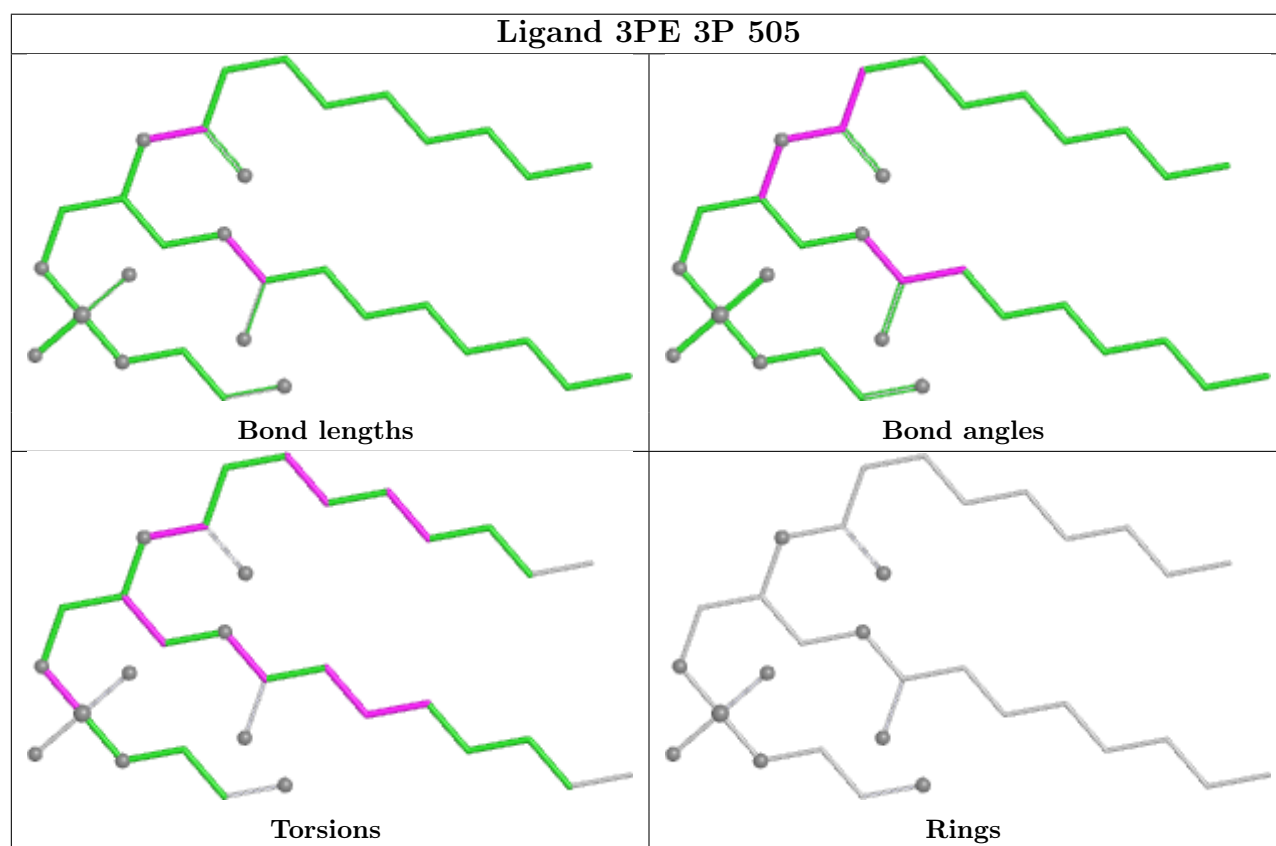
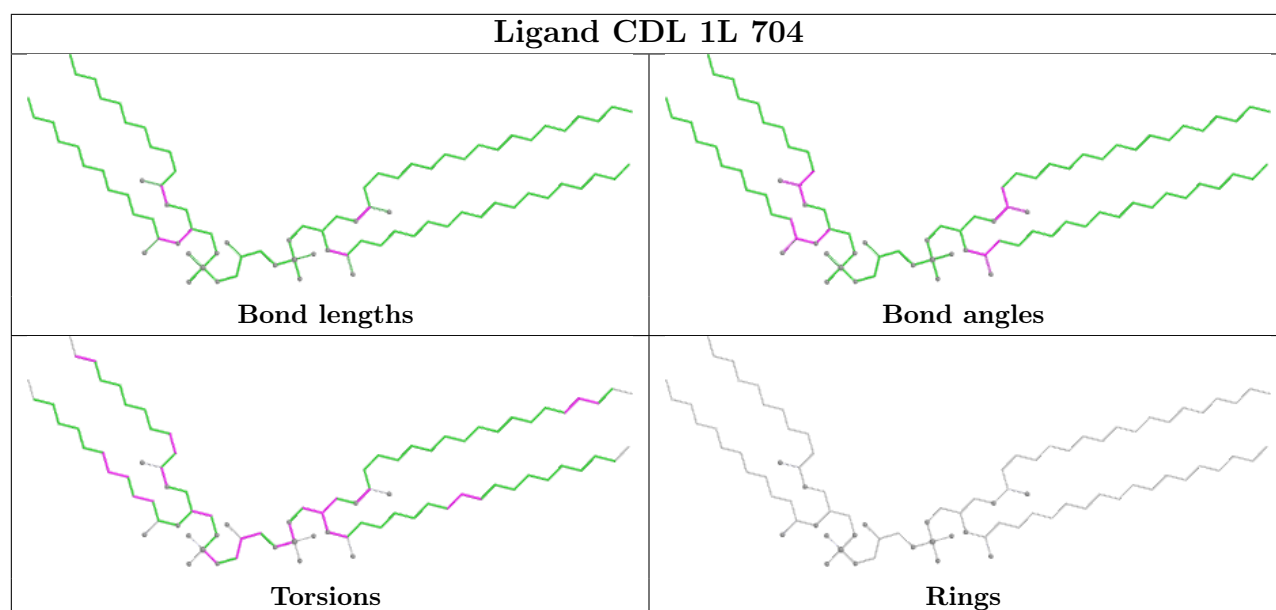


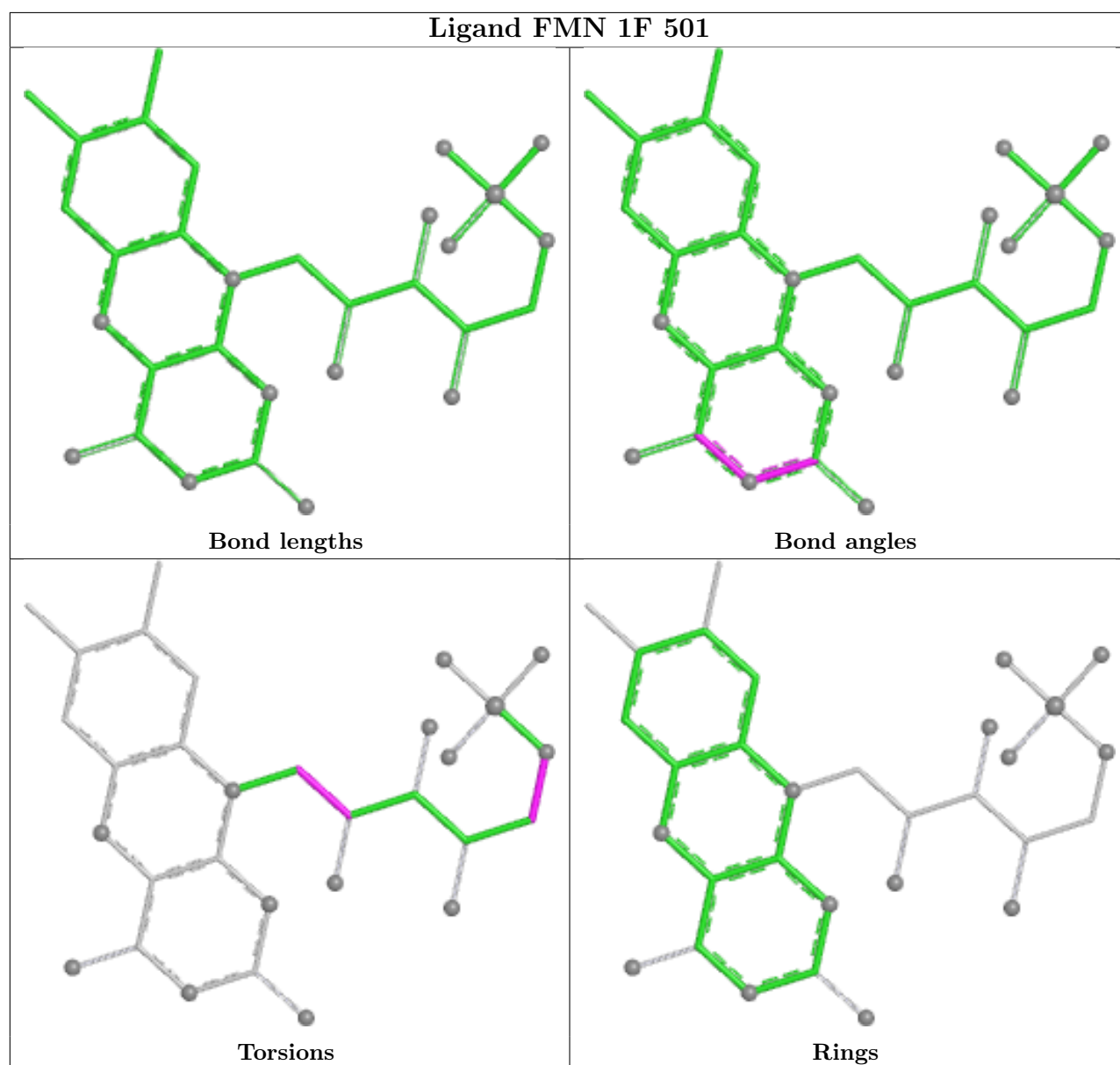
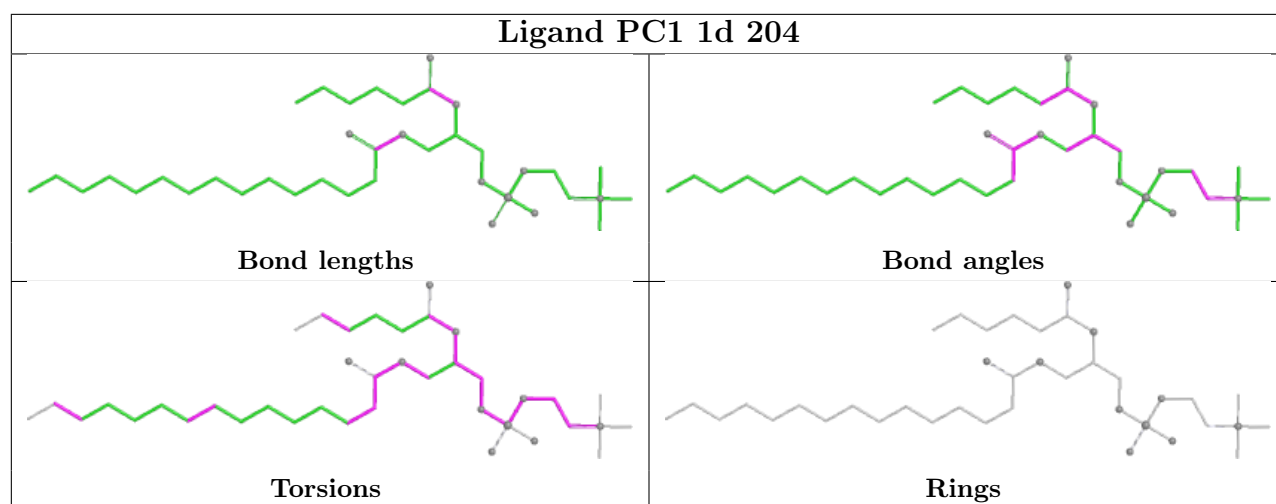


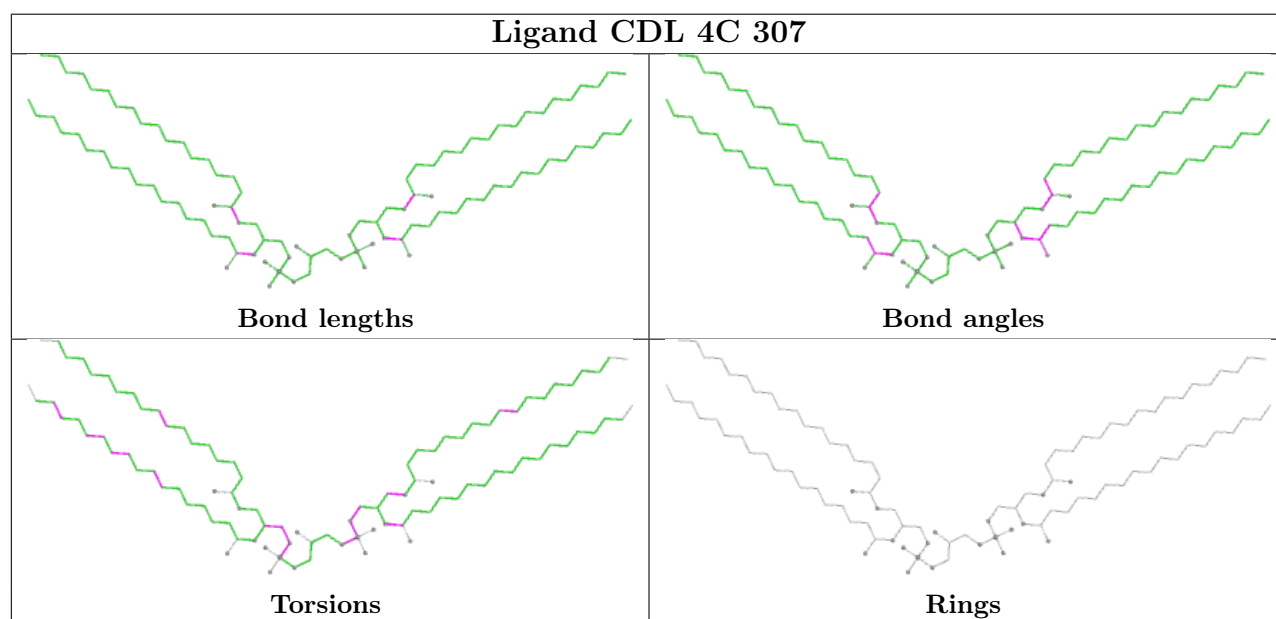
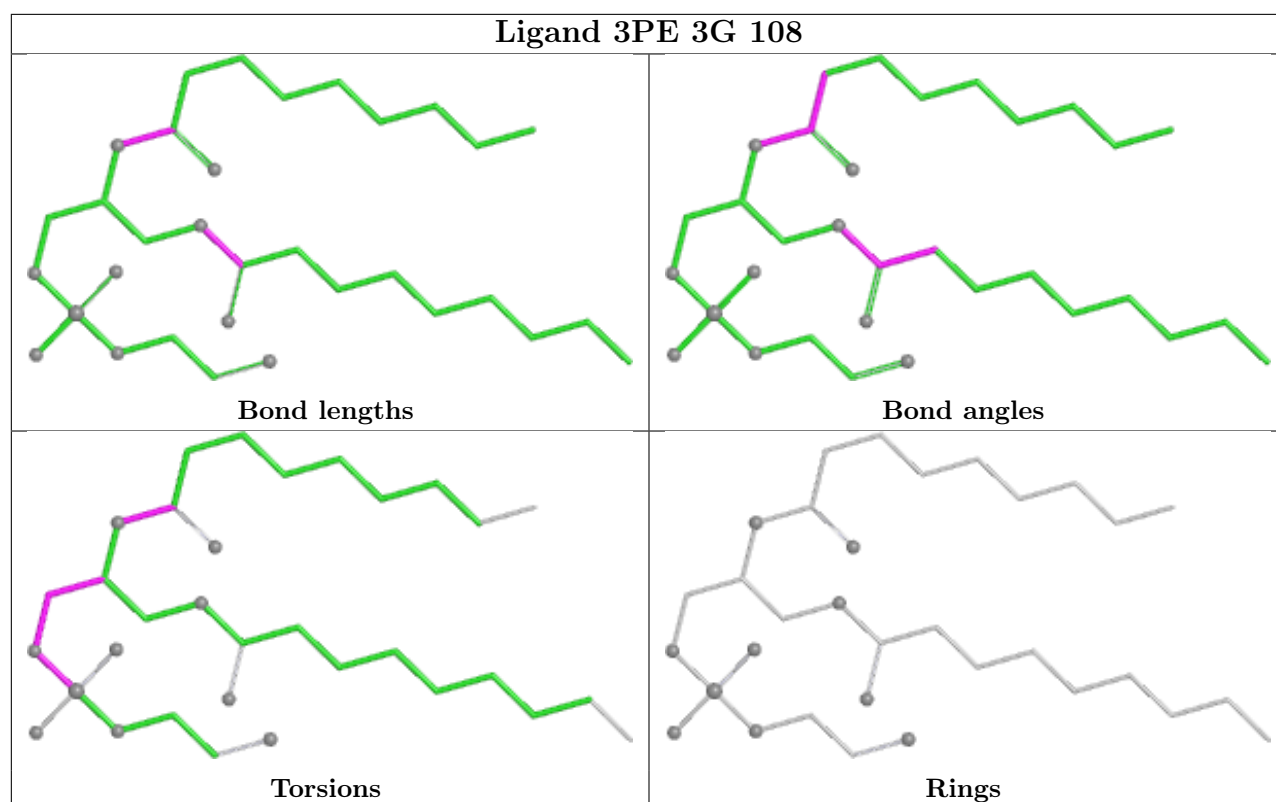


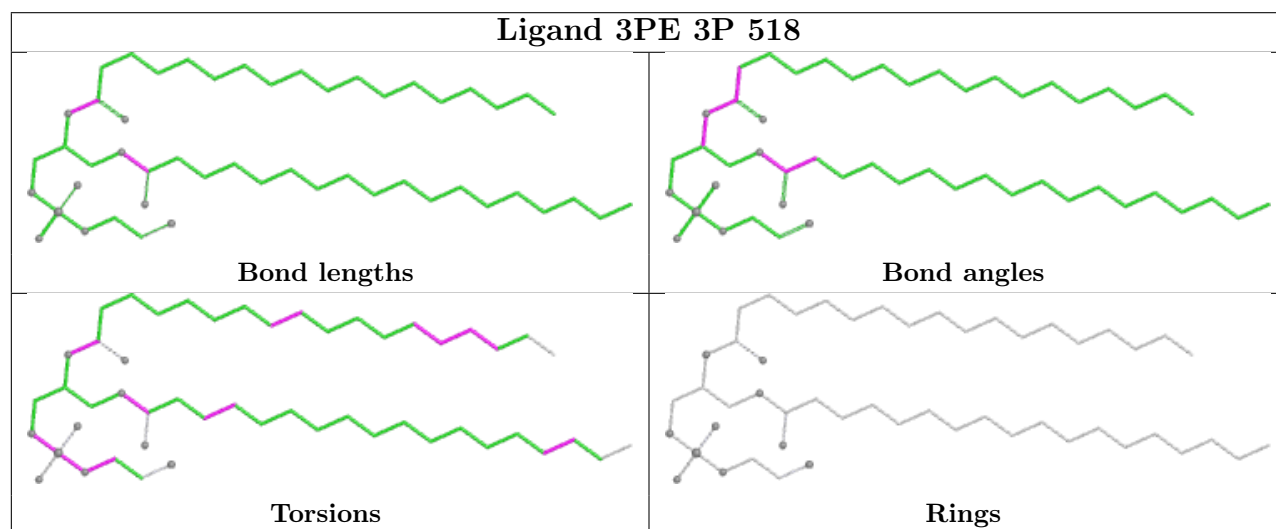
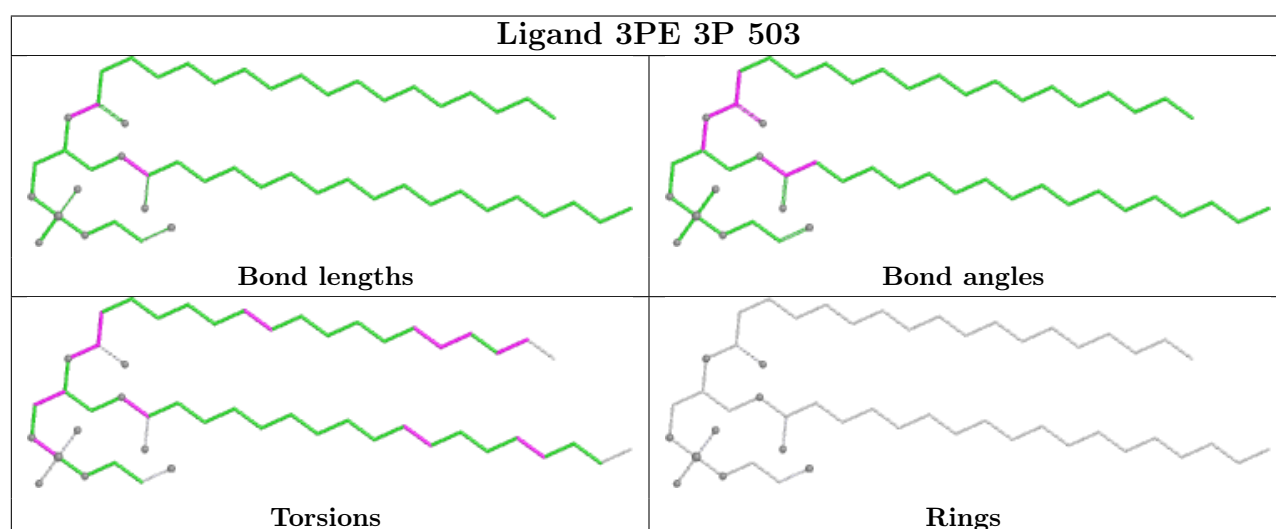
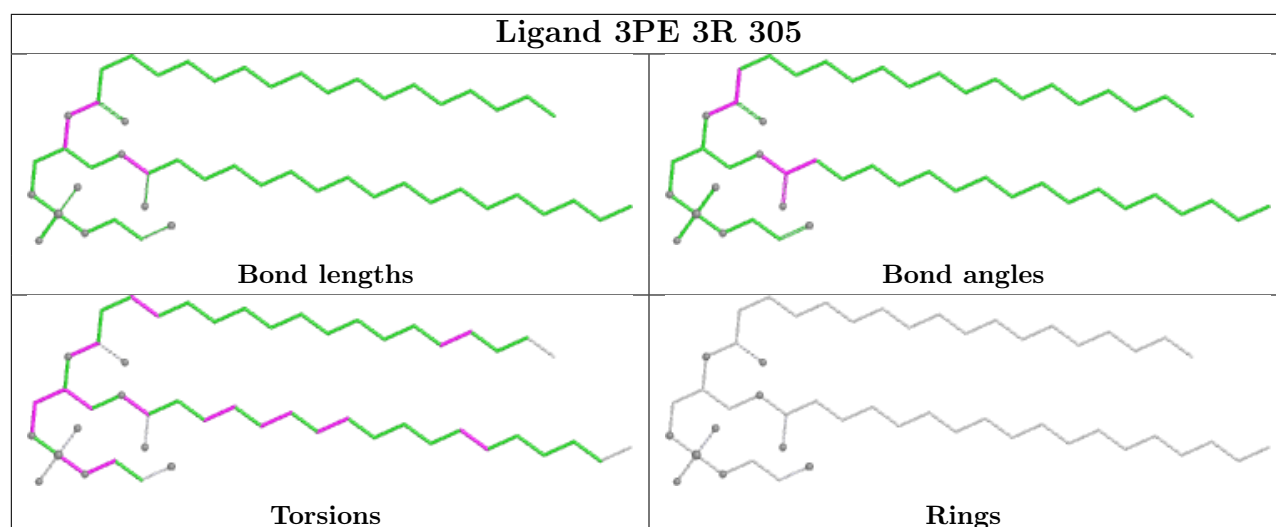


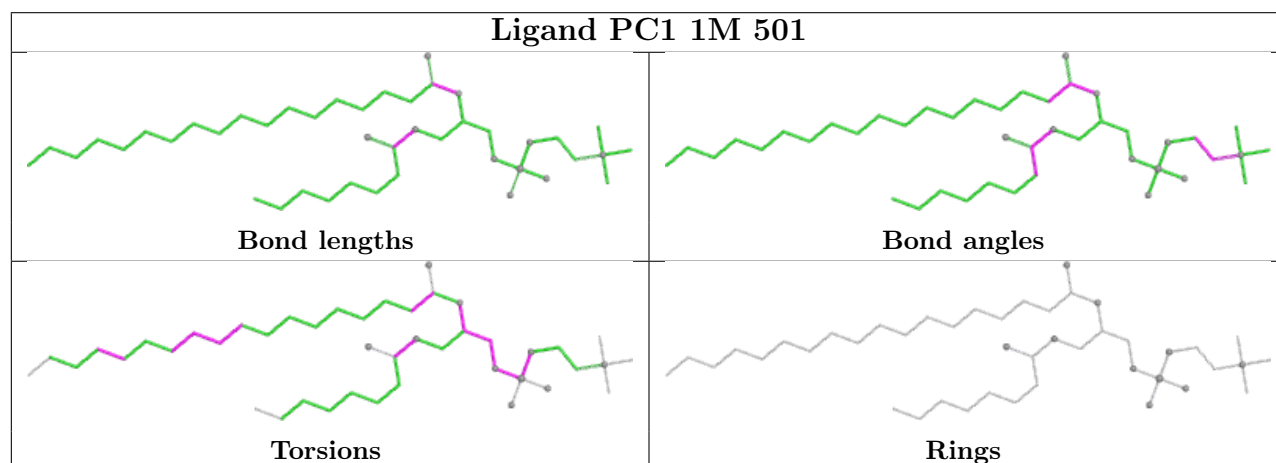
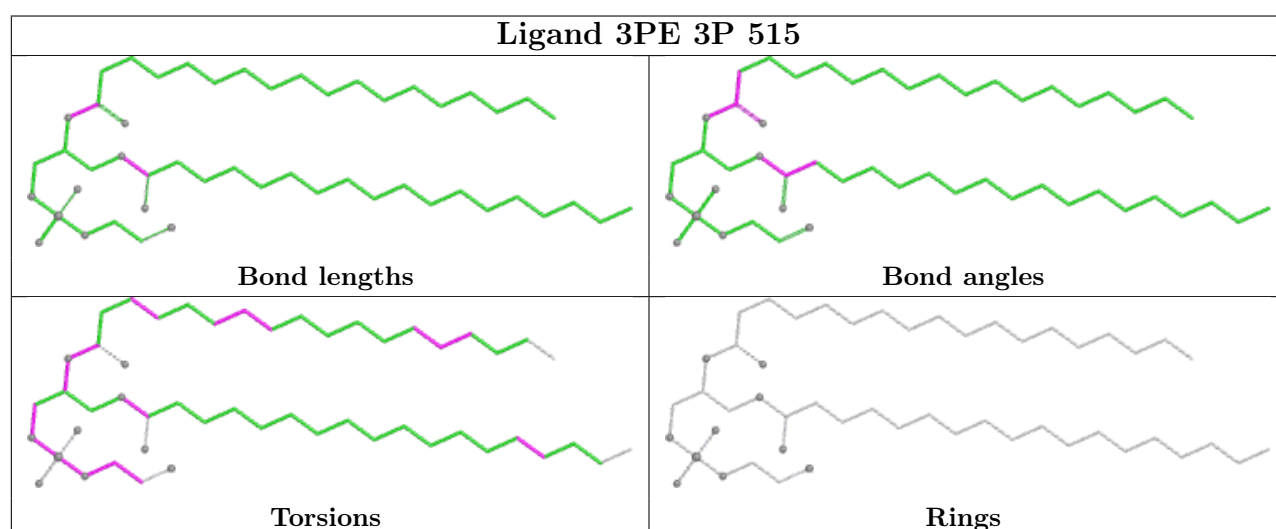
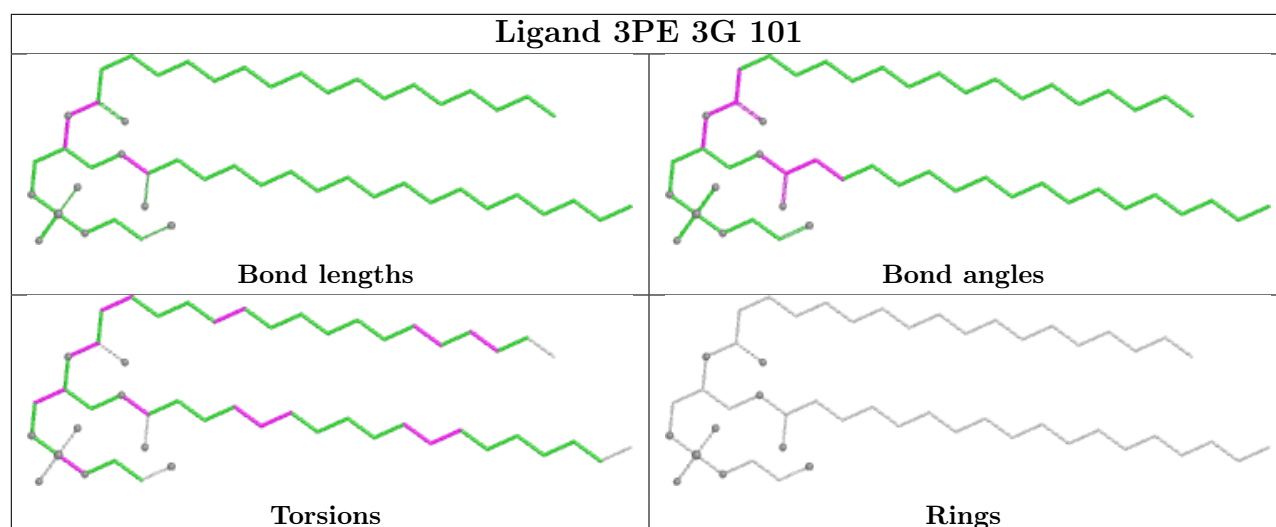


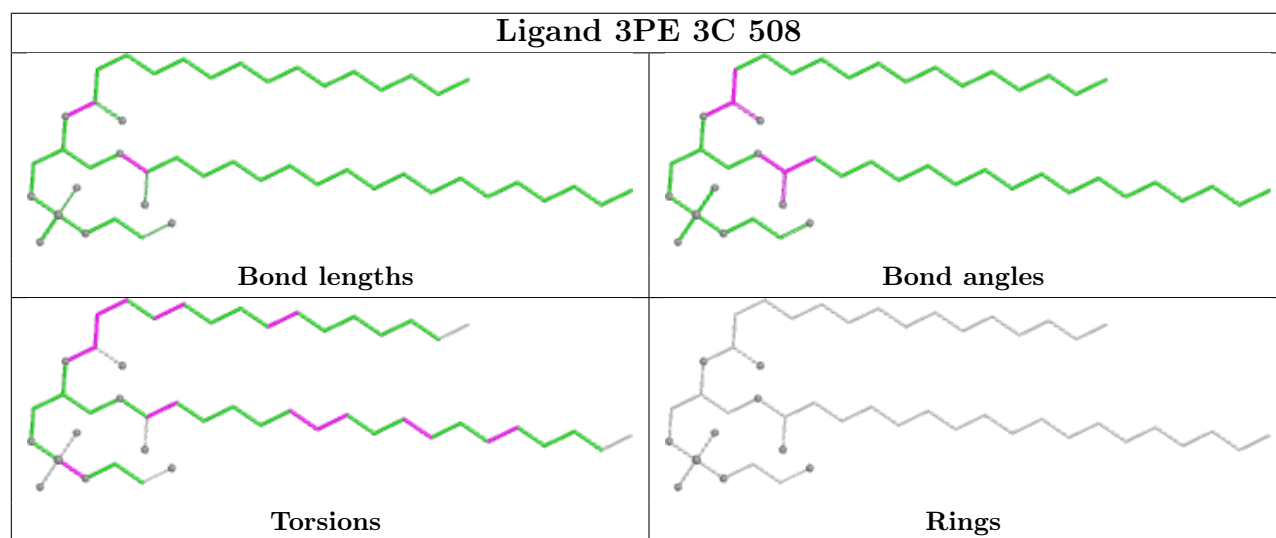
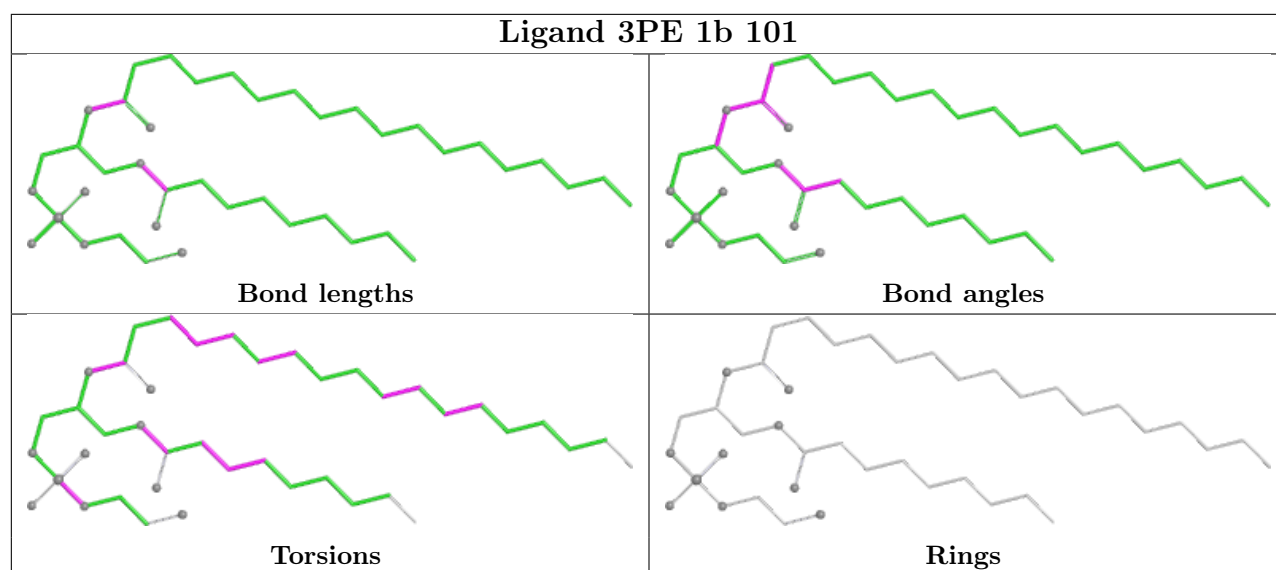


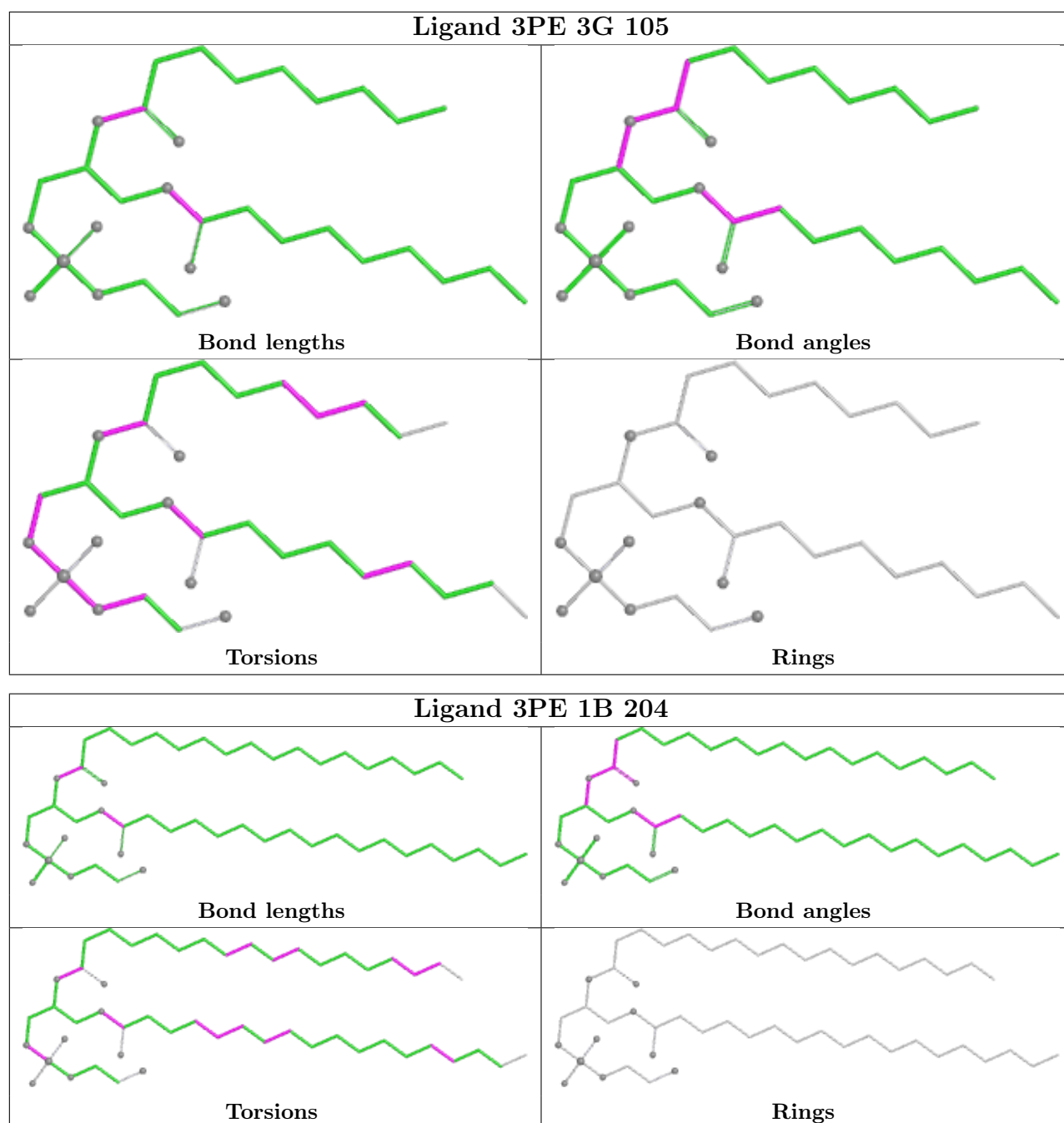


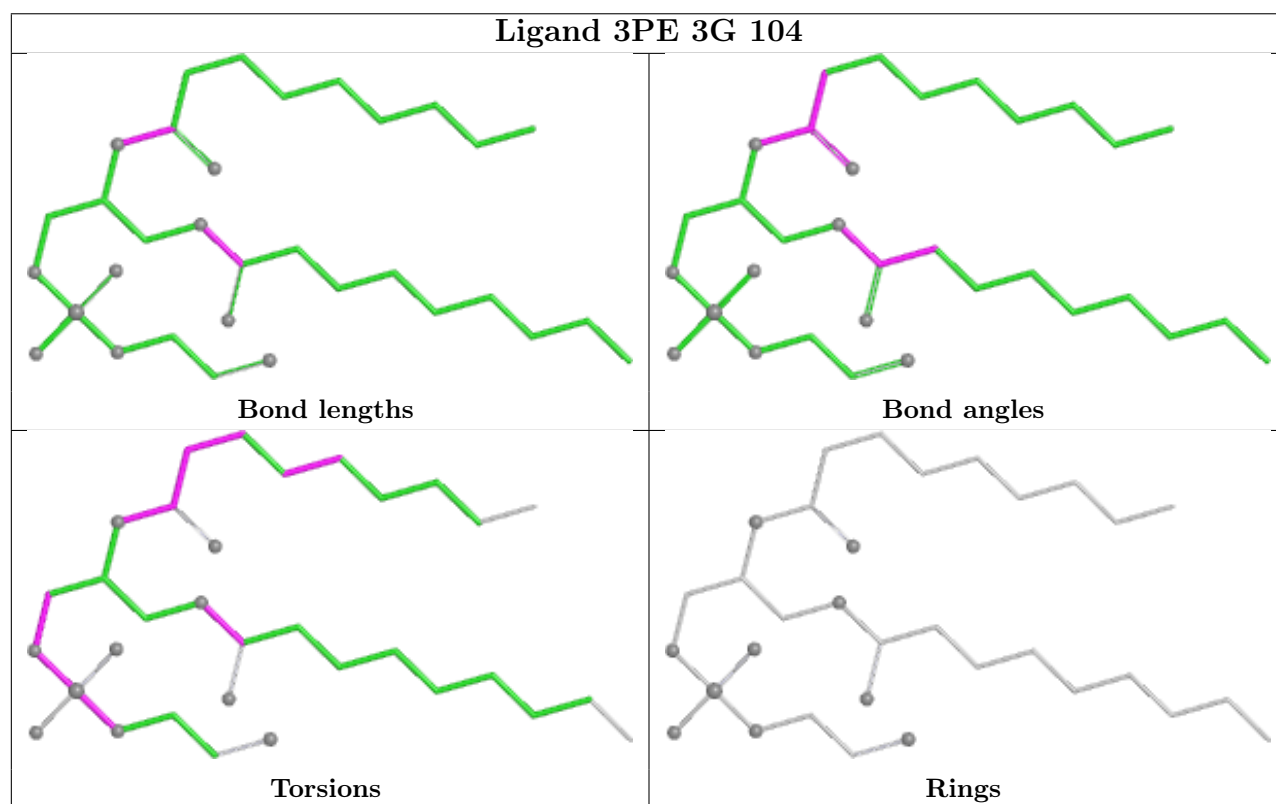
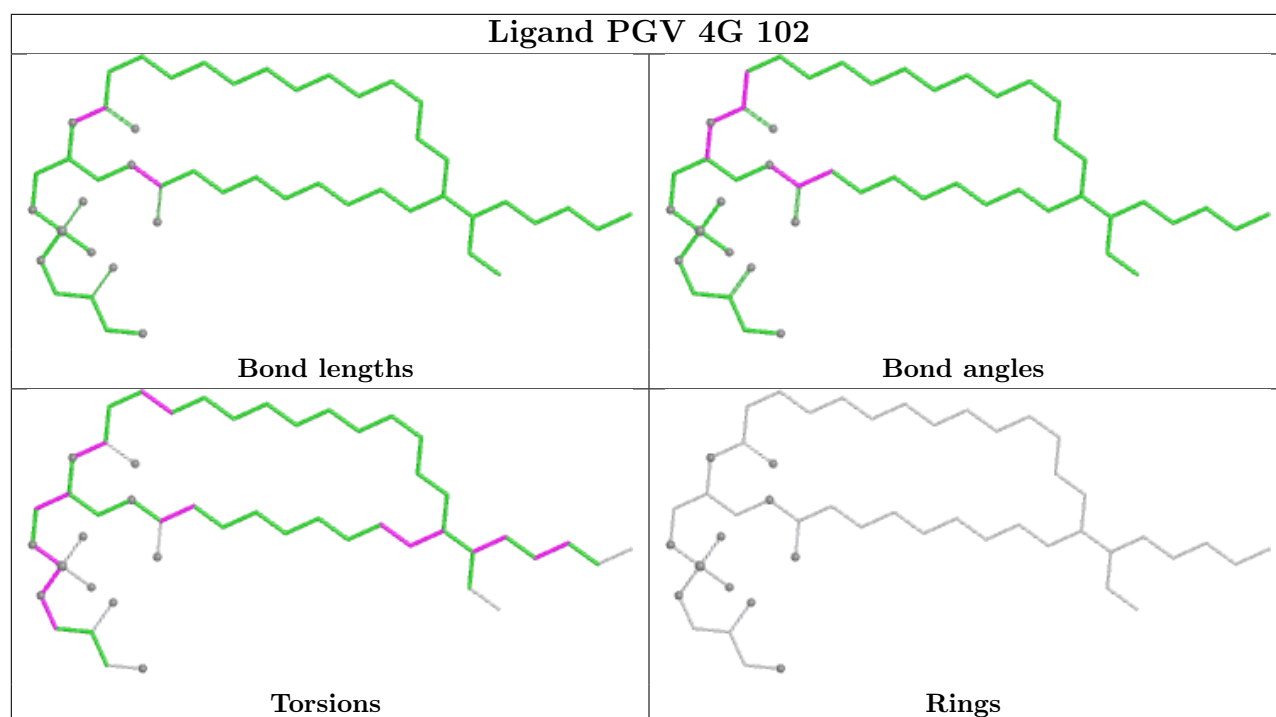


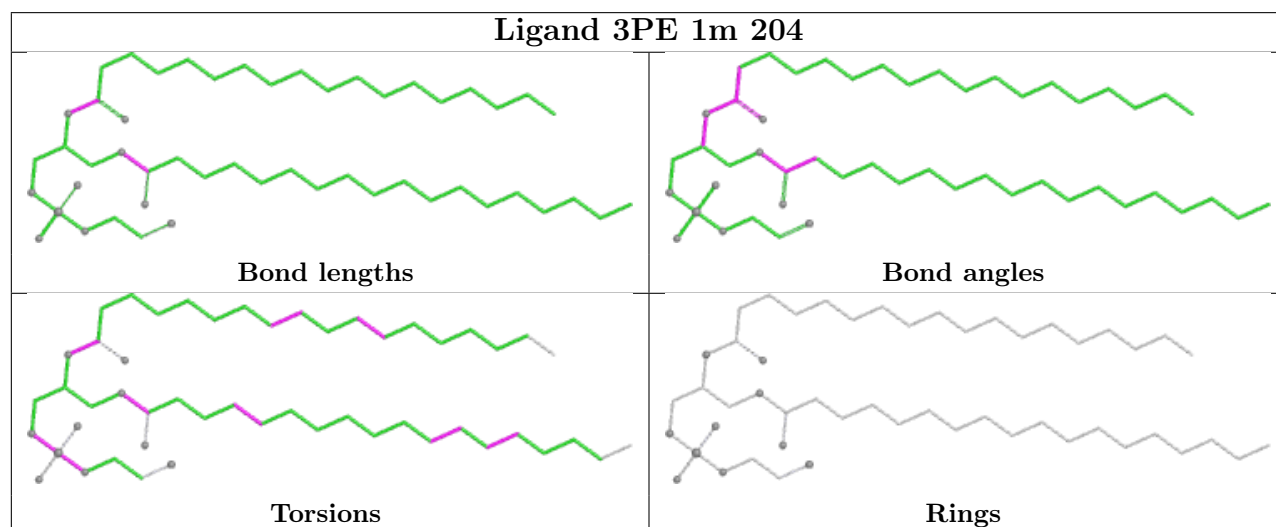
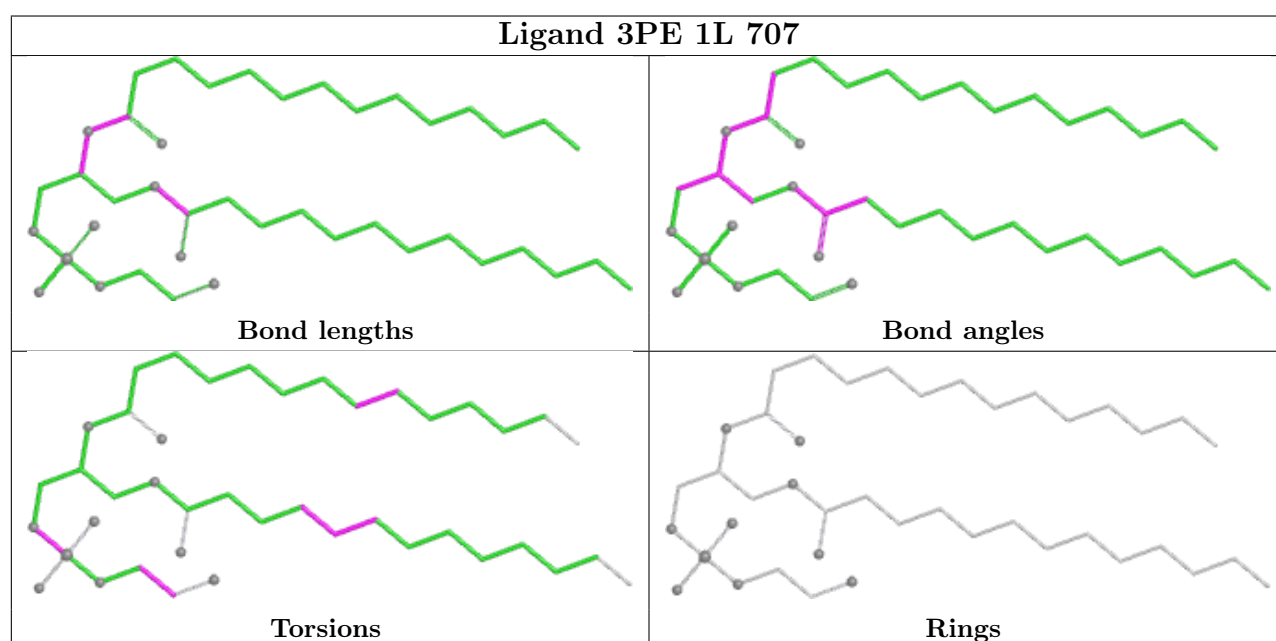
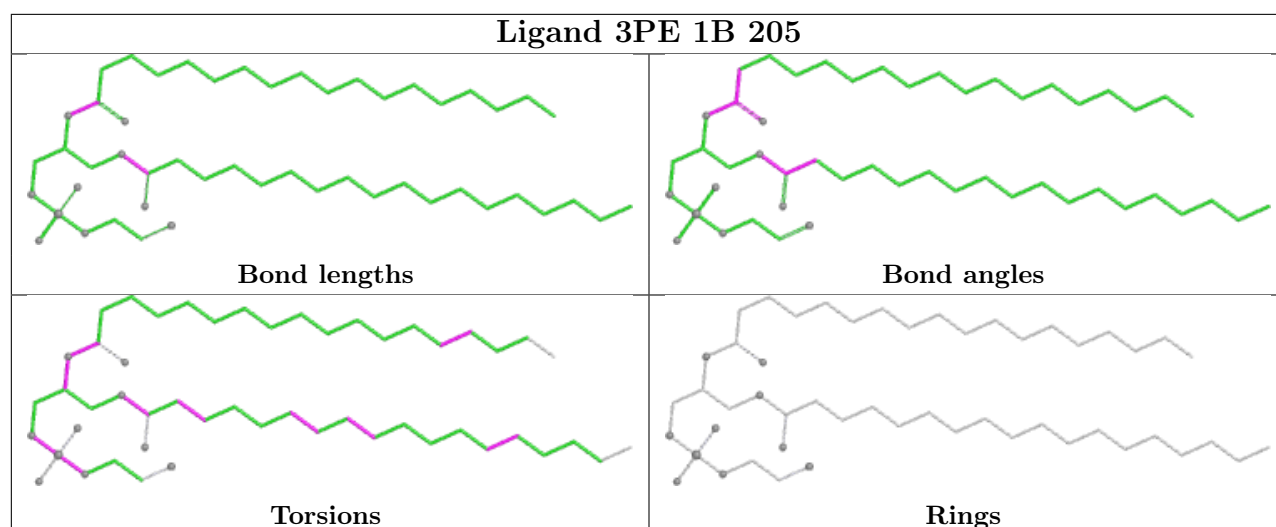


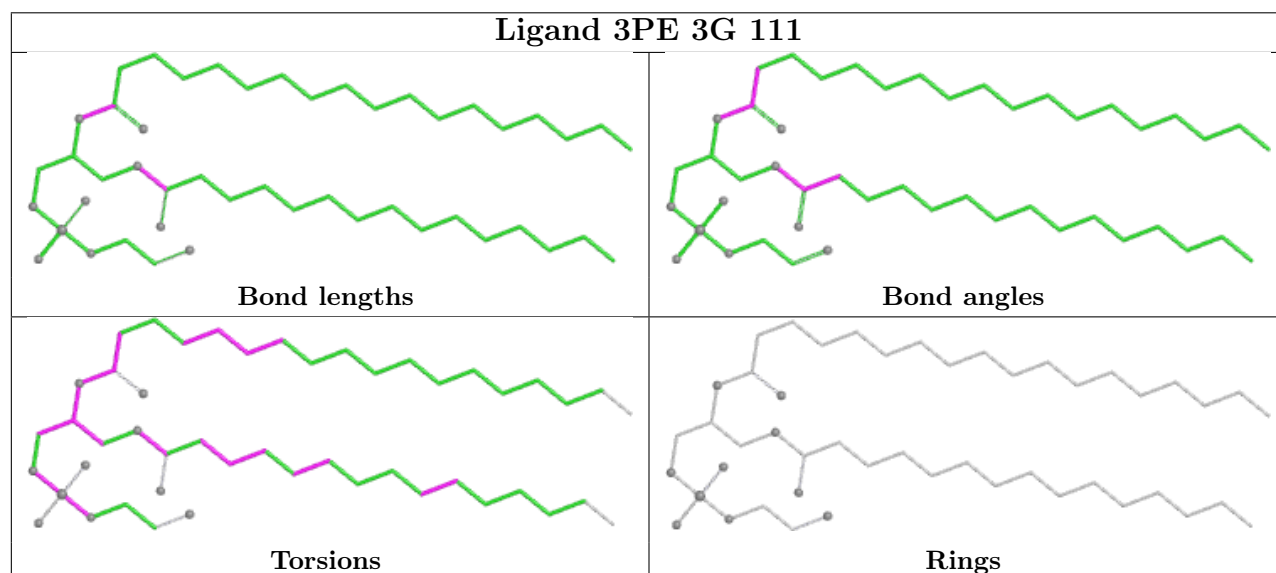
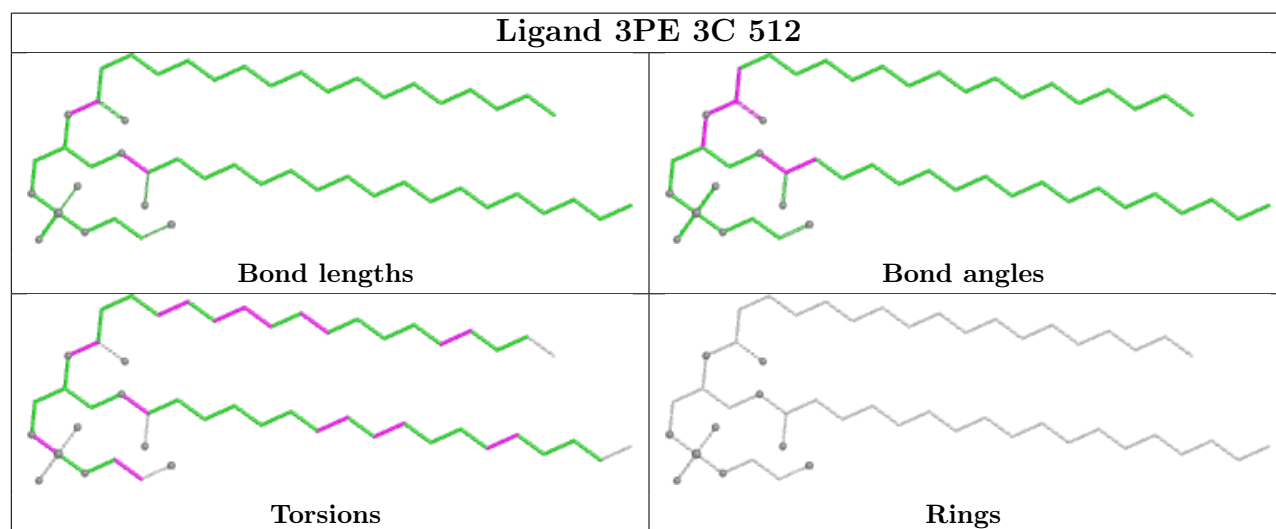
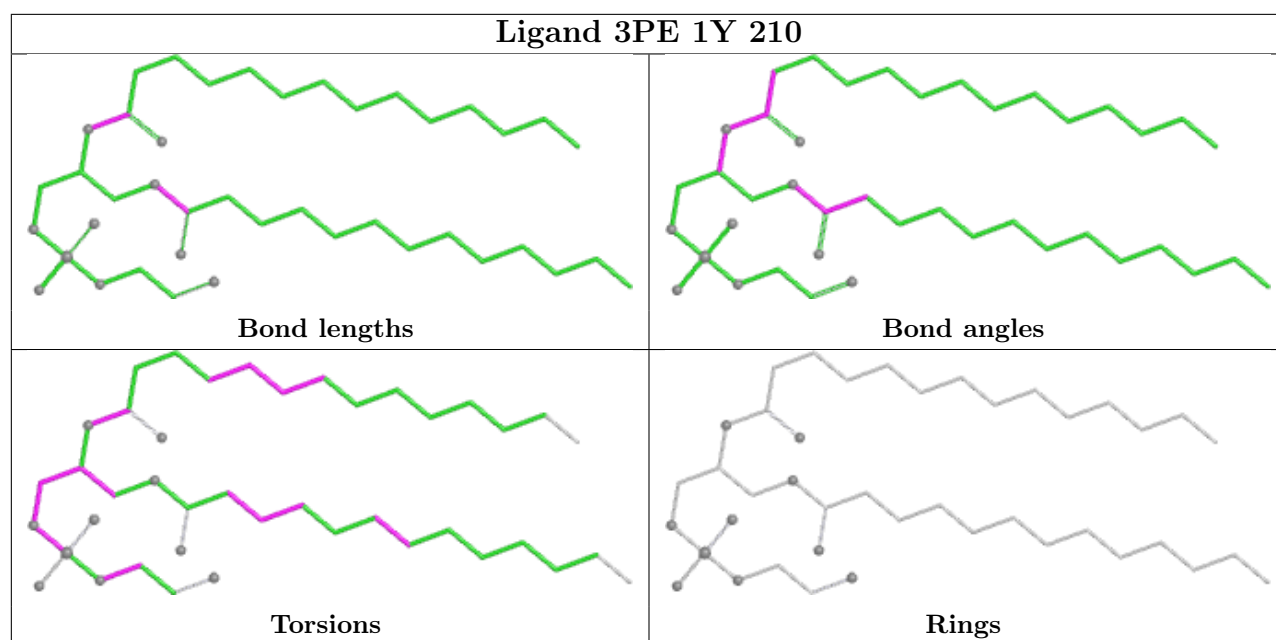




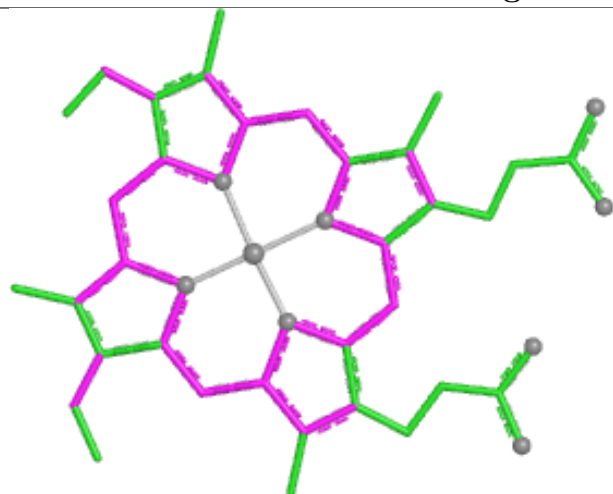




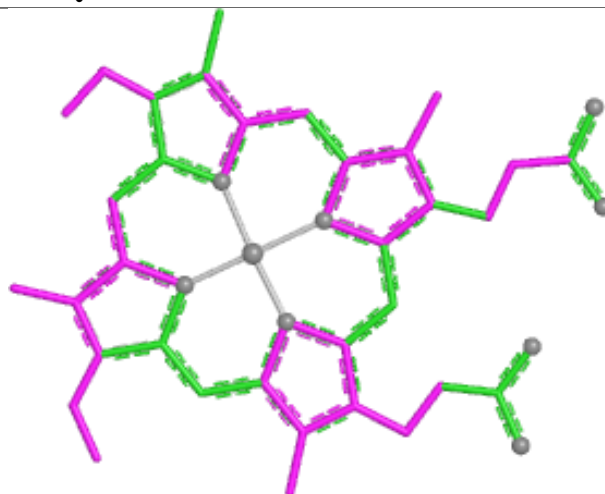




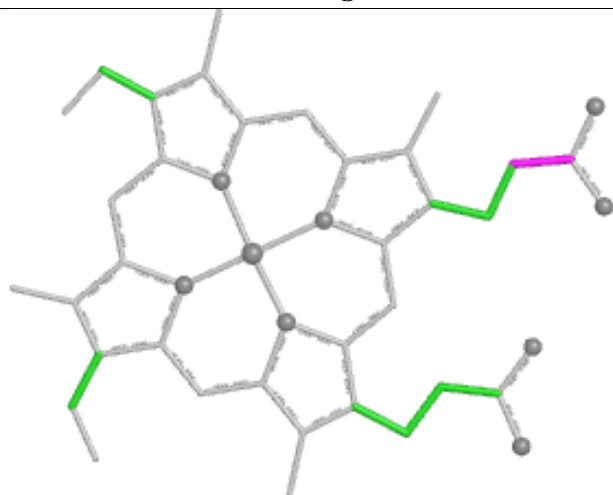
Ligand HEC 3Q 501



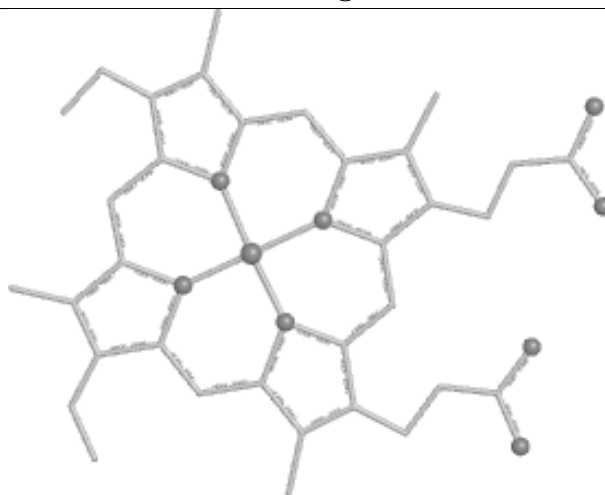
Bond lengths



Bond angles

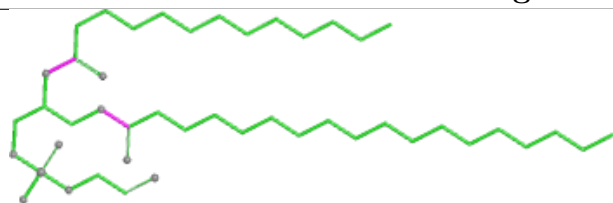


Torsions

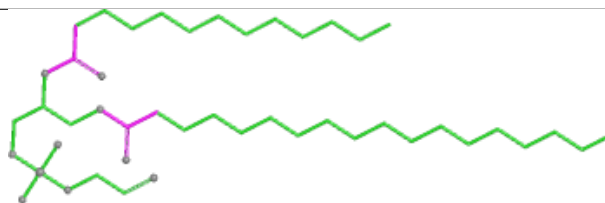


Rings

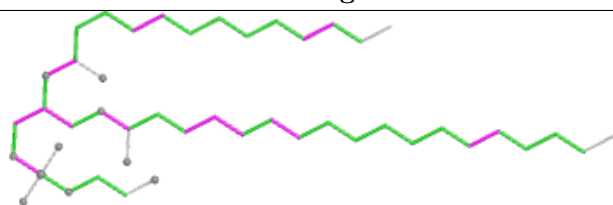
Ligand 3PE 1k 101



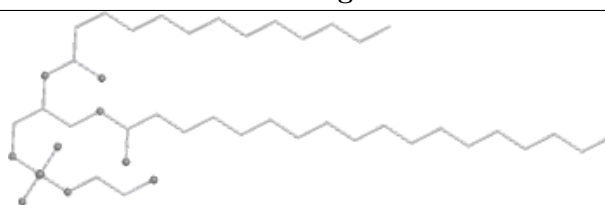
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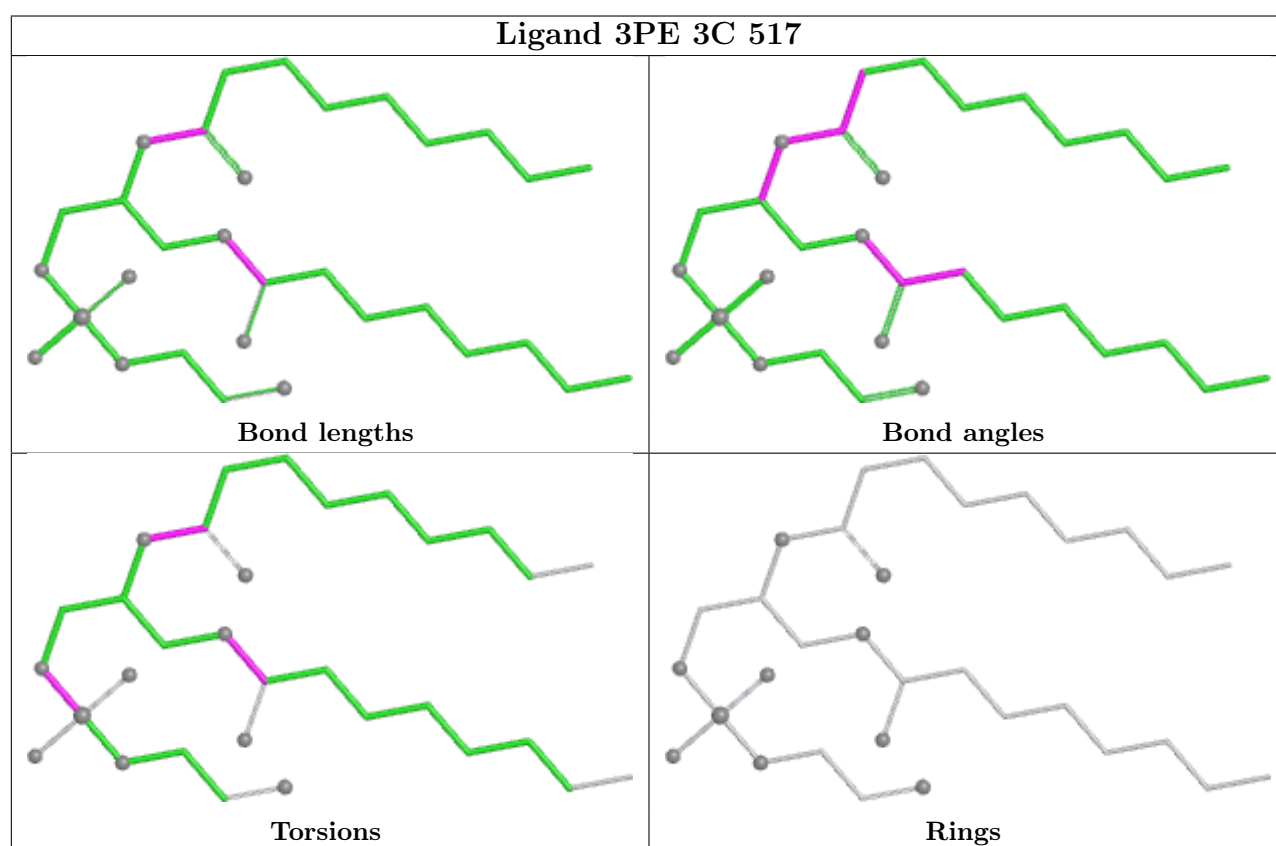
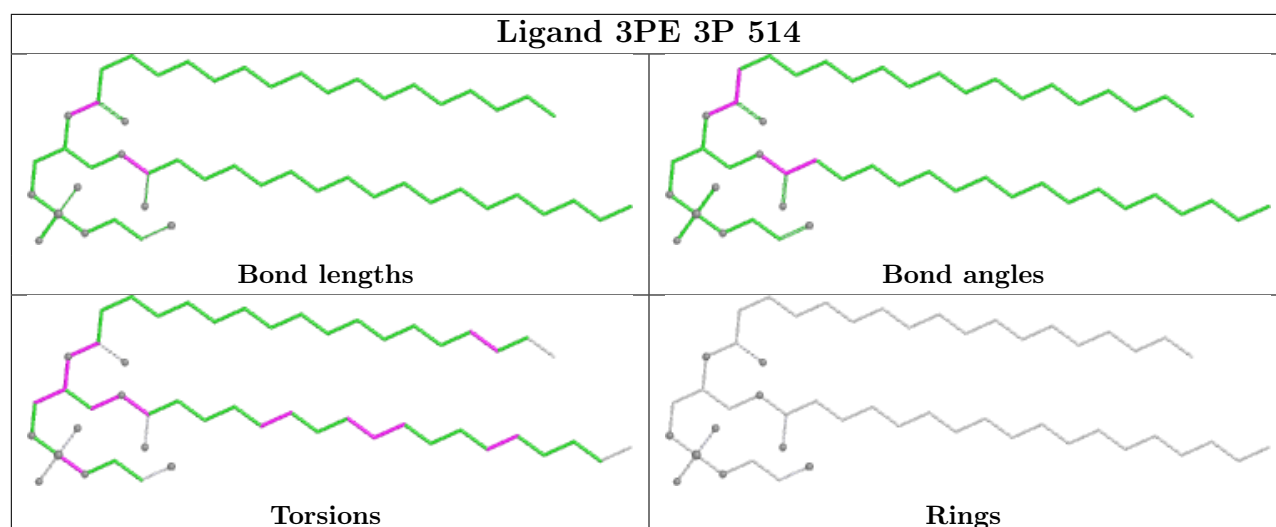
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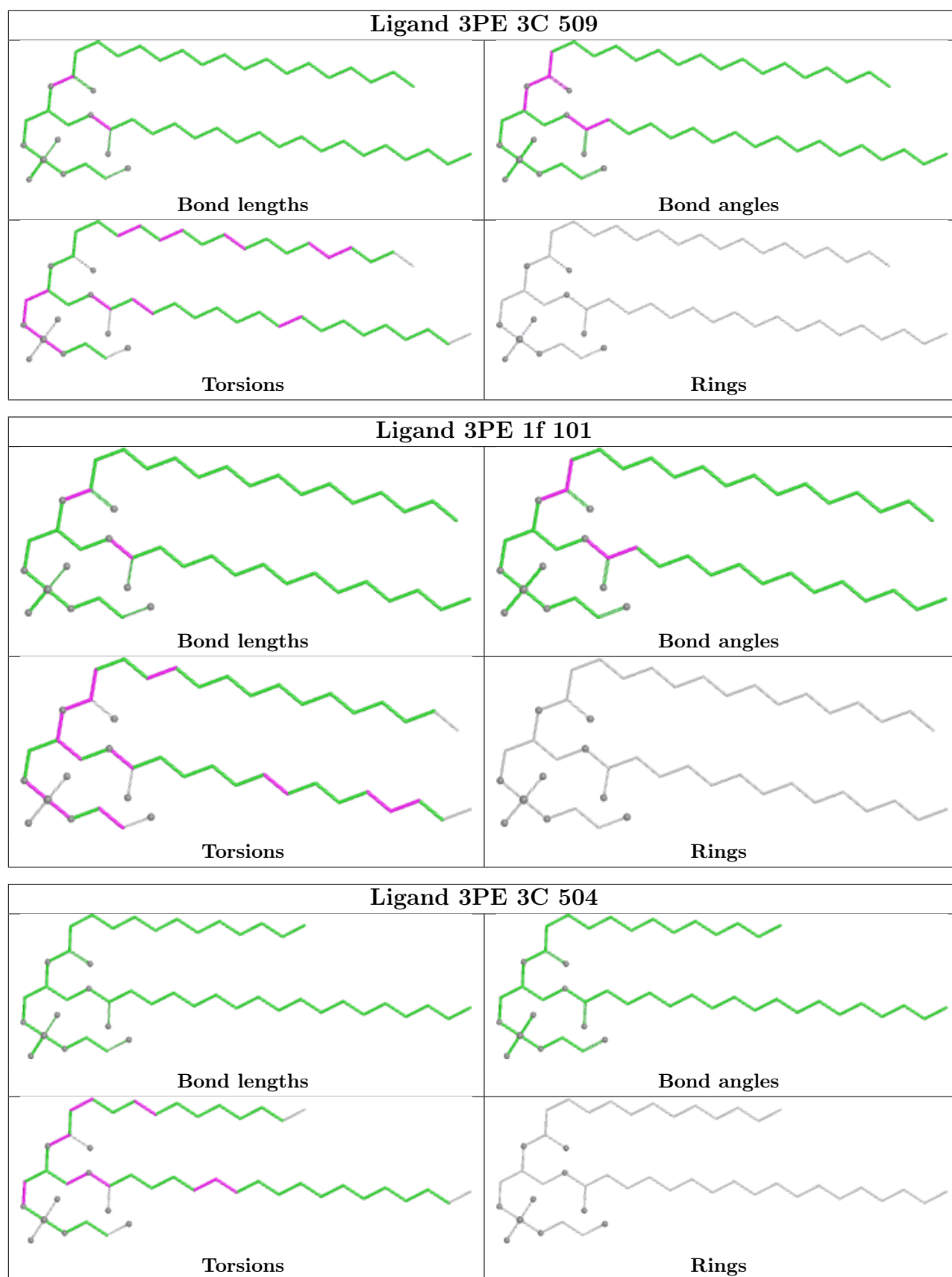


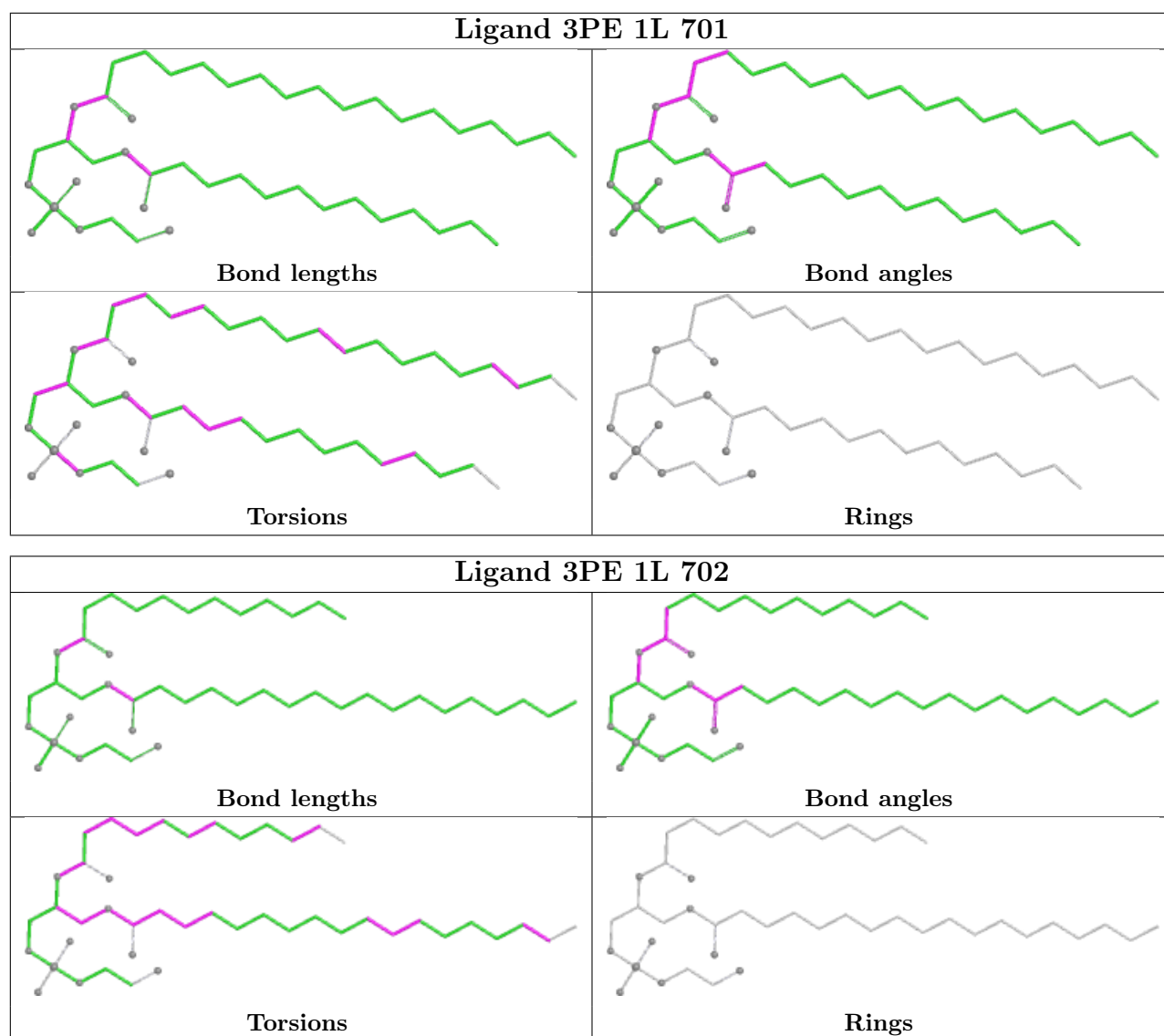
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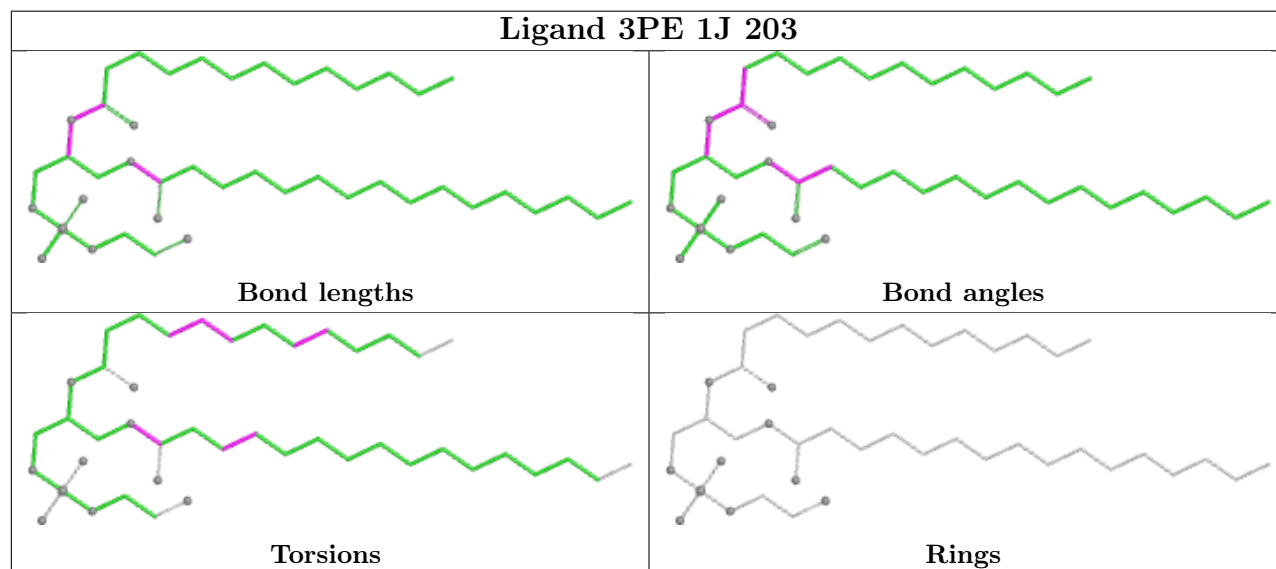
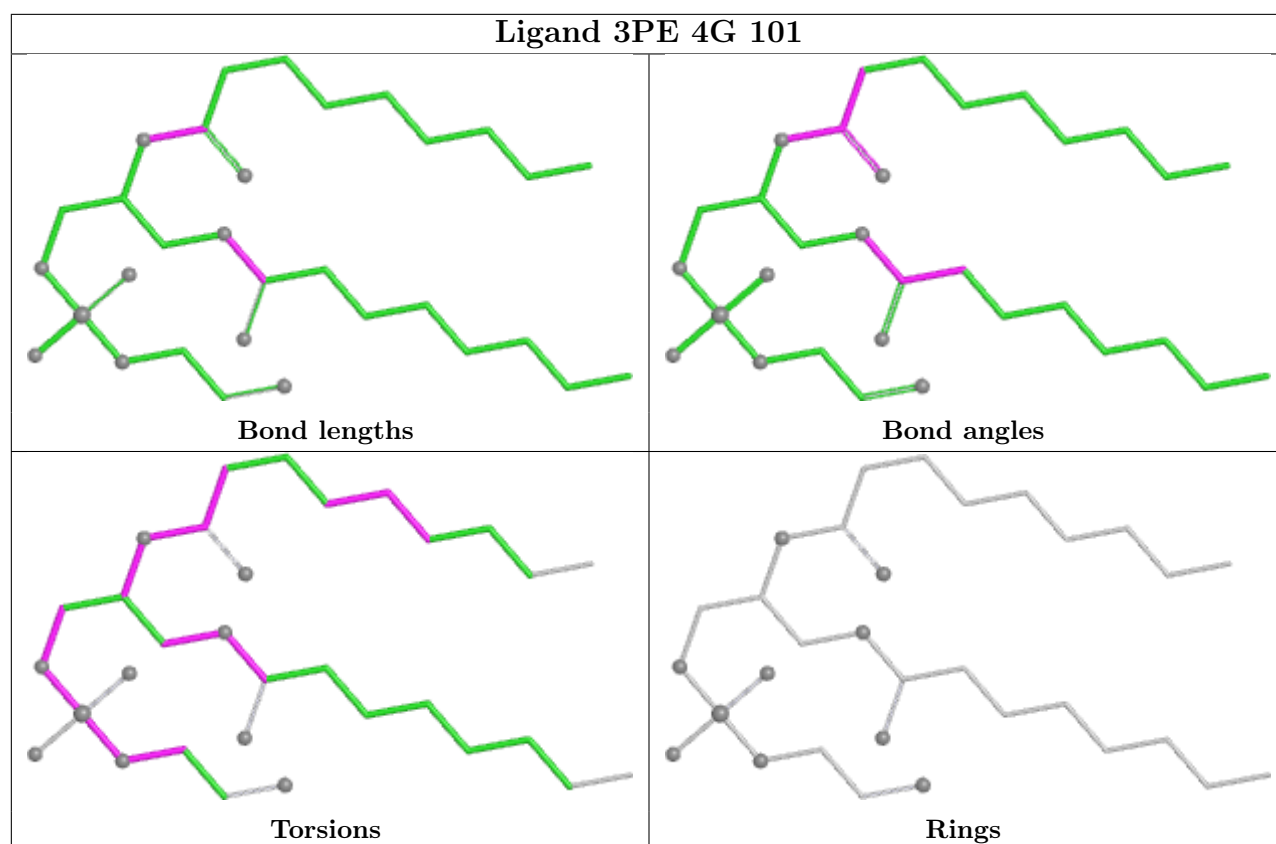


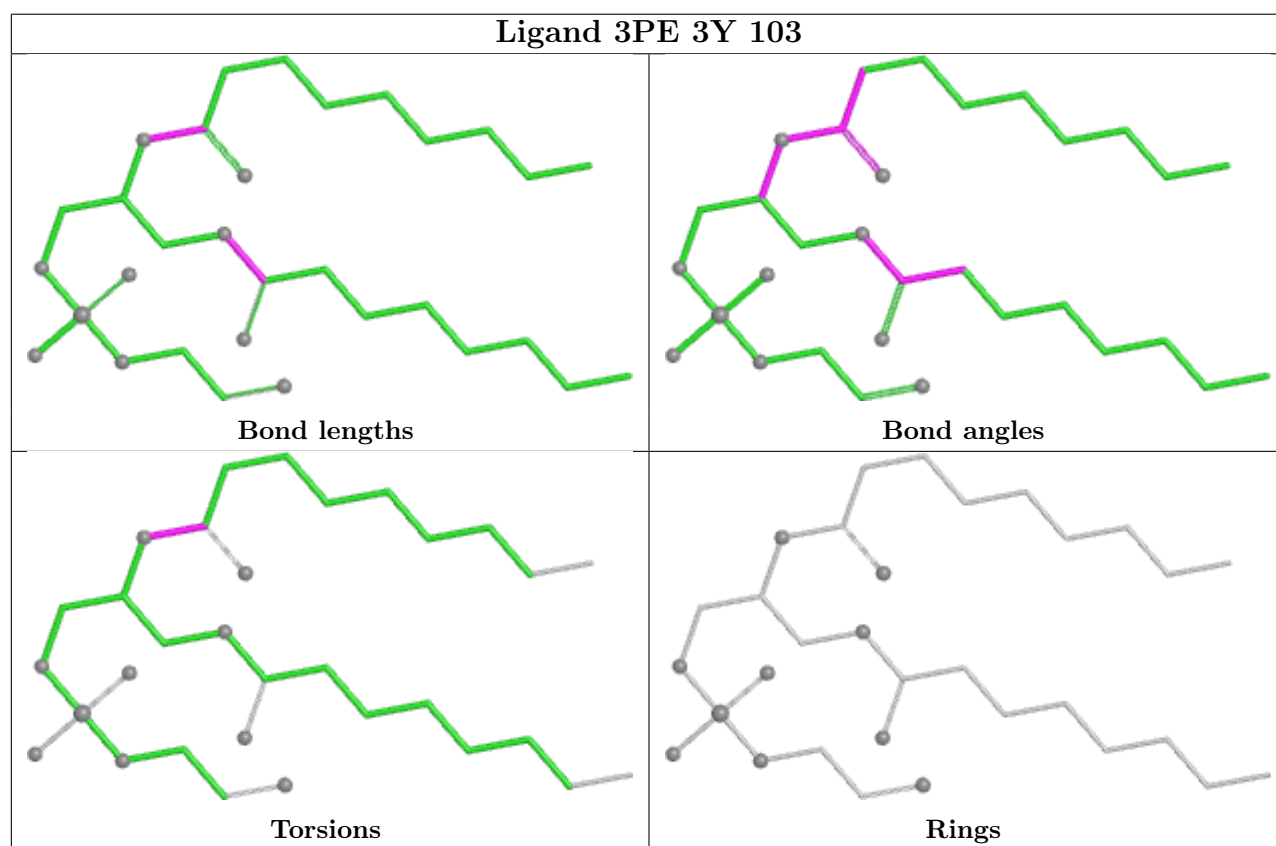
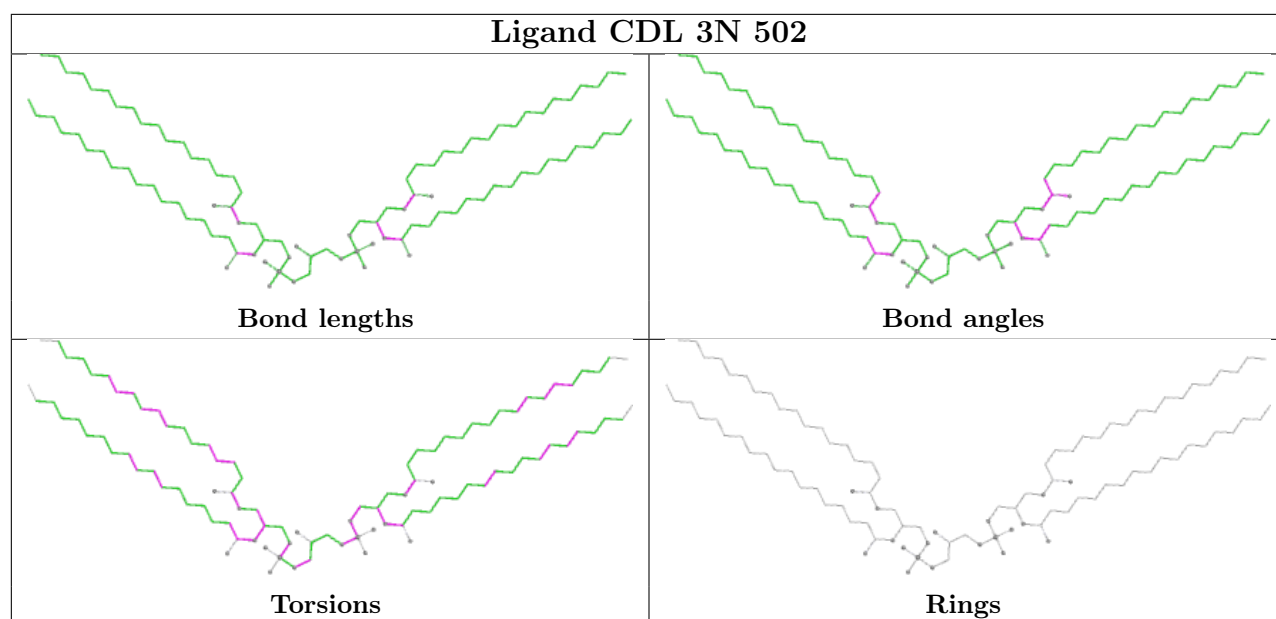
Rings

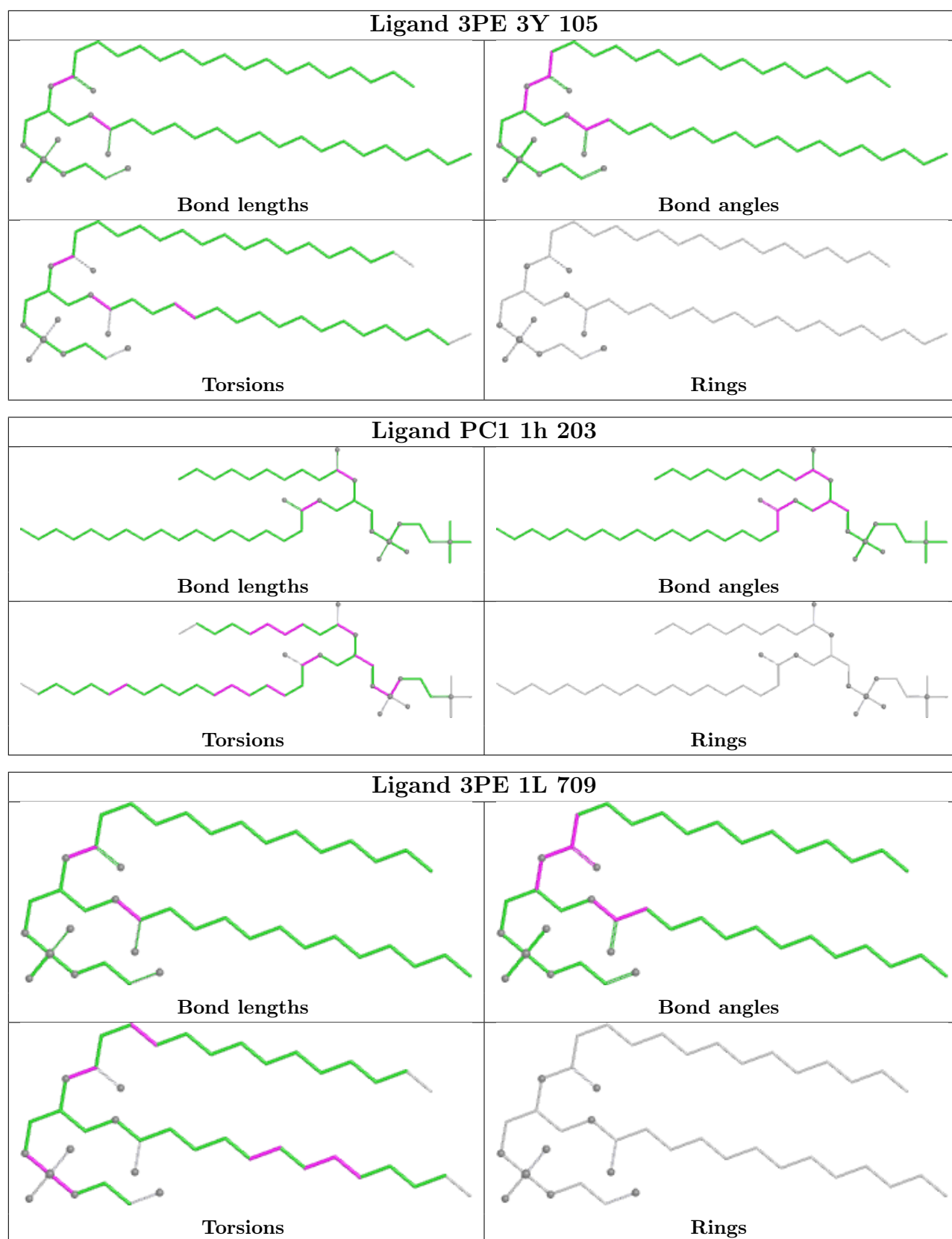


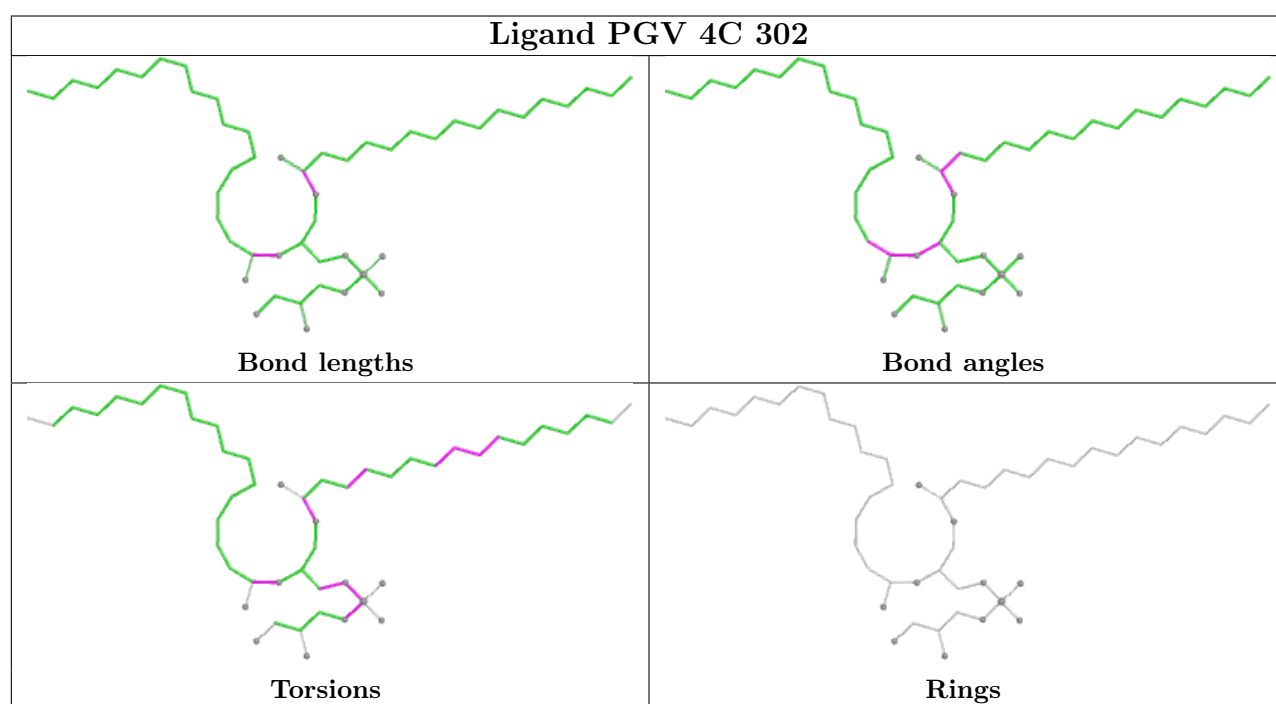
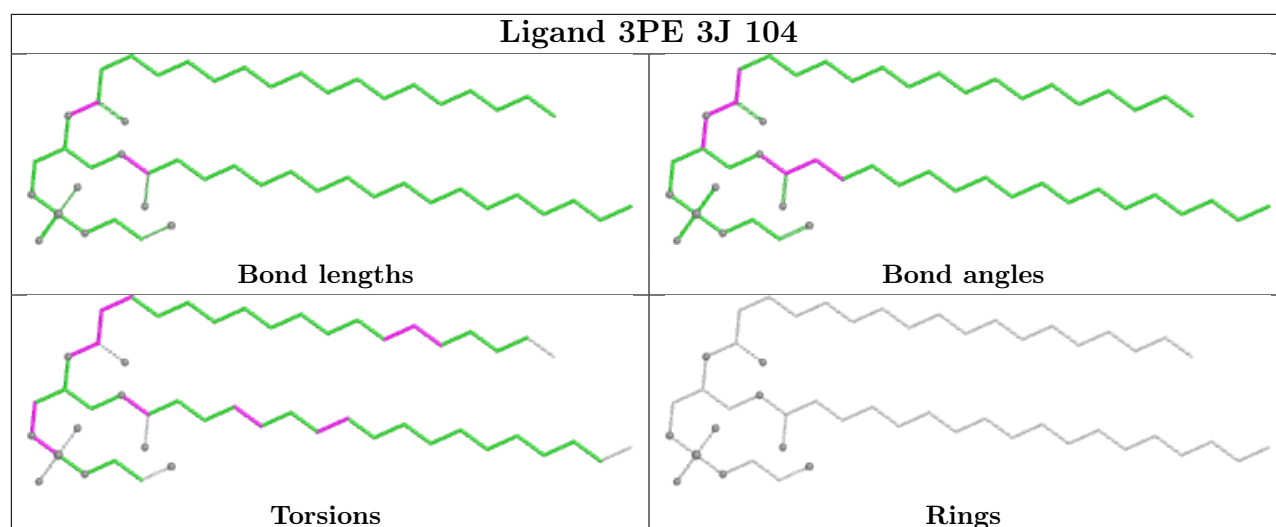


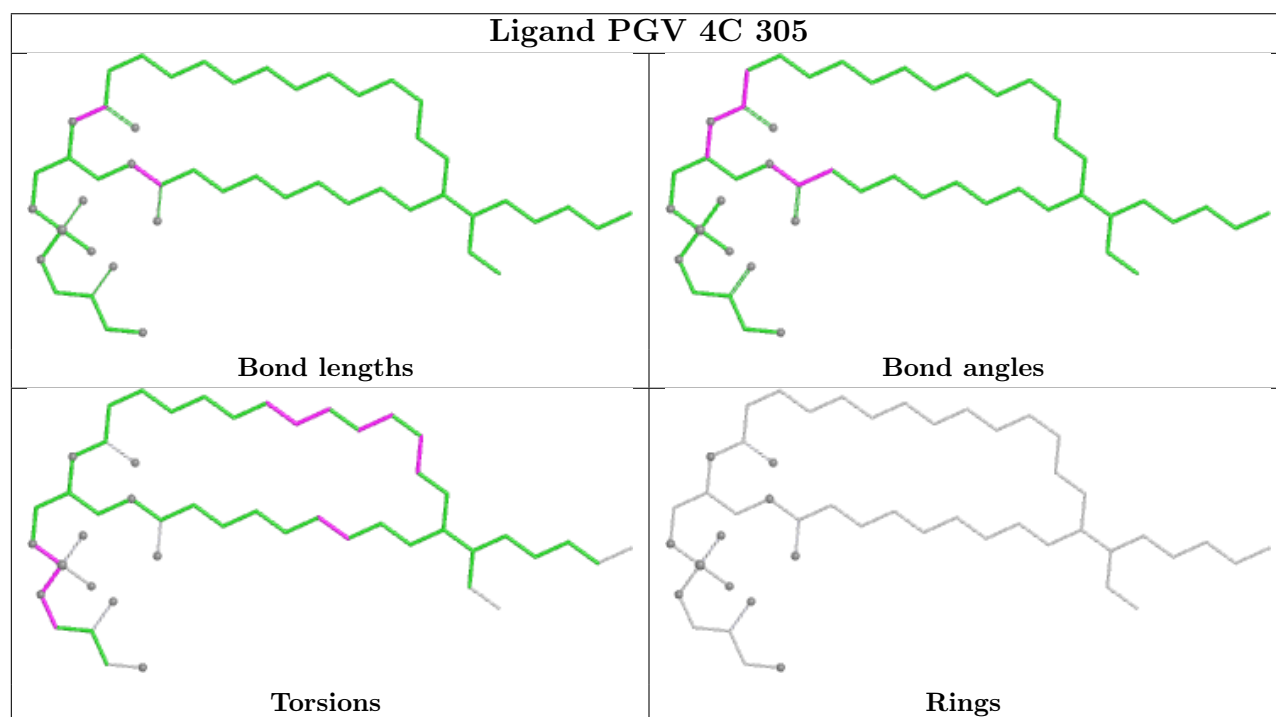
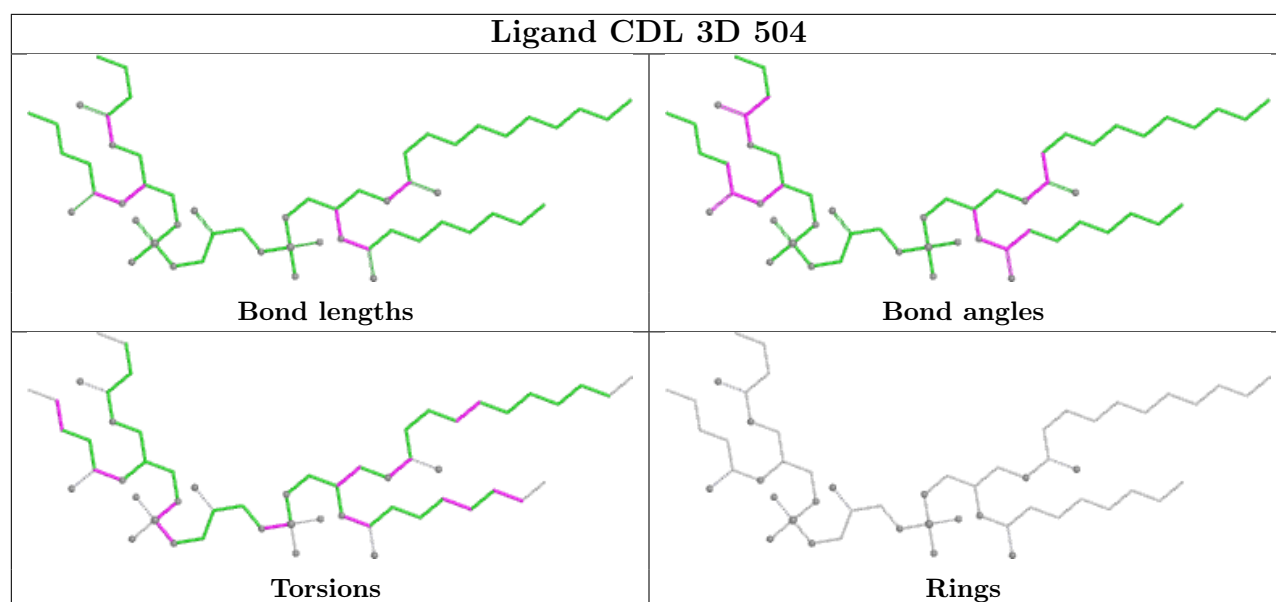


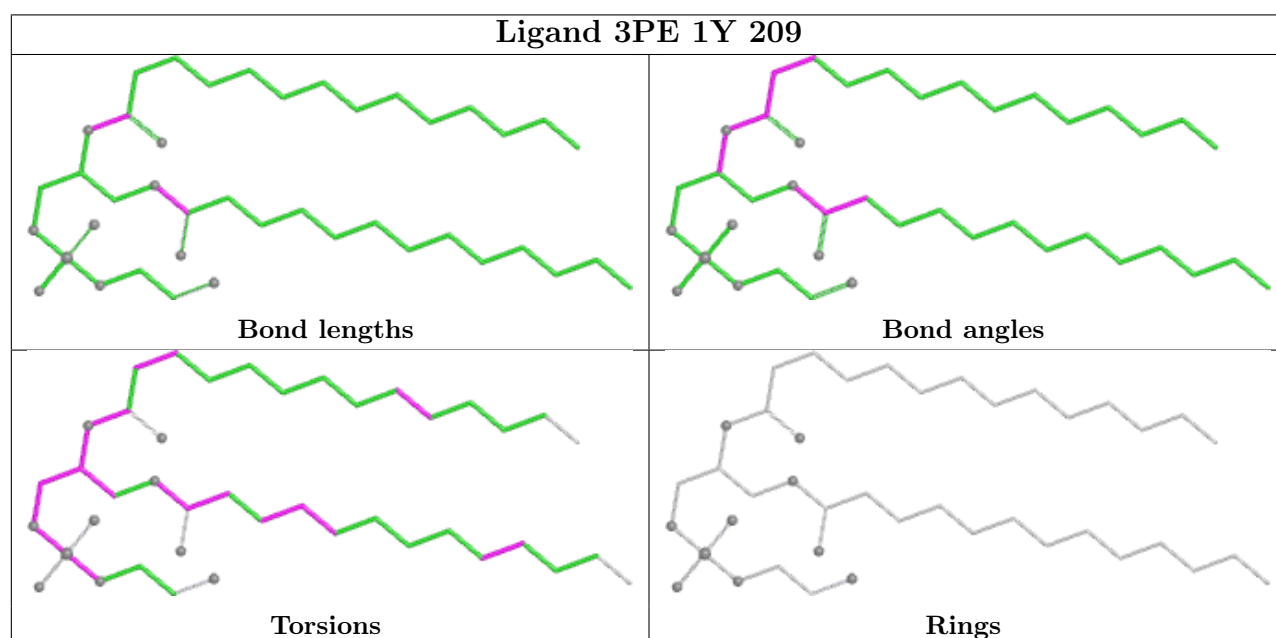
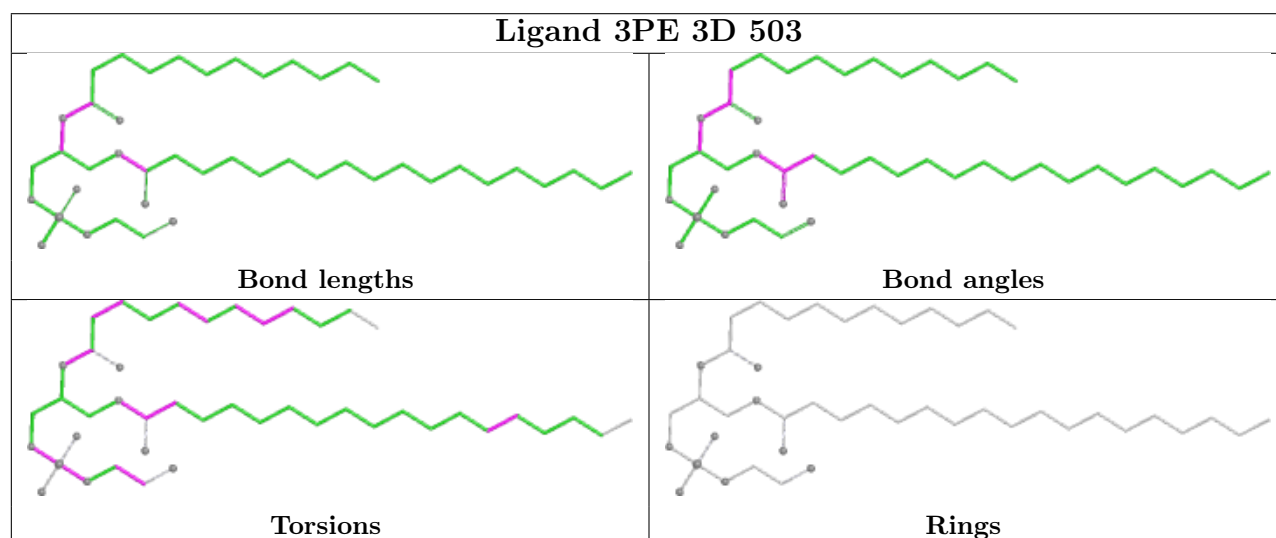
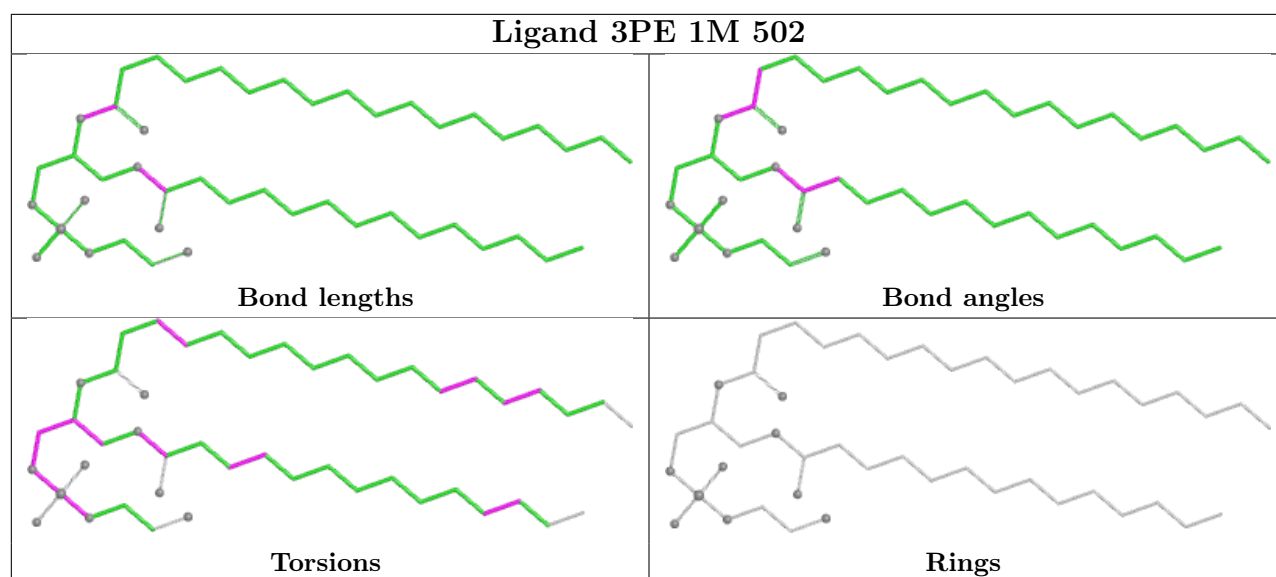


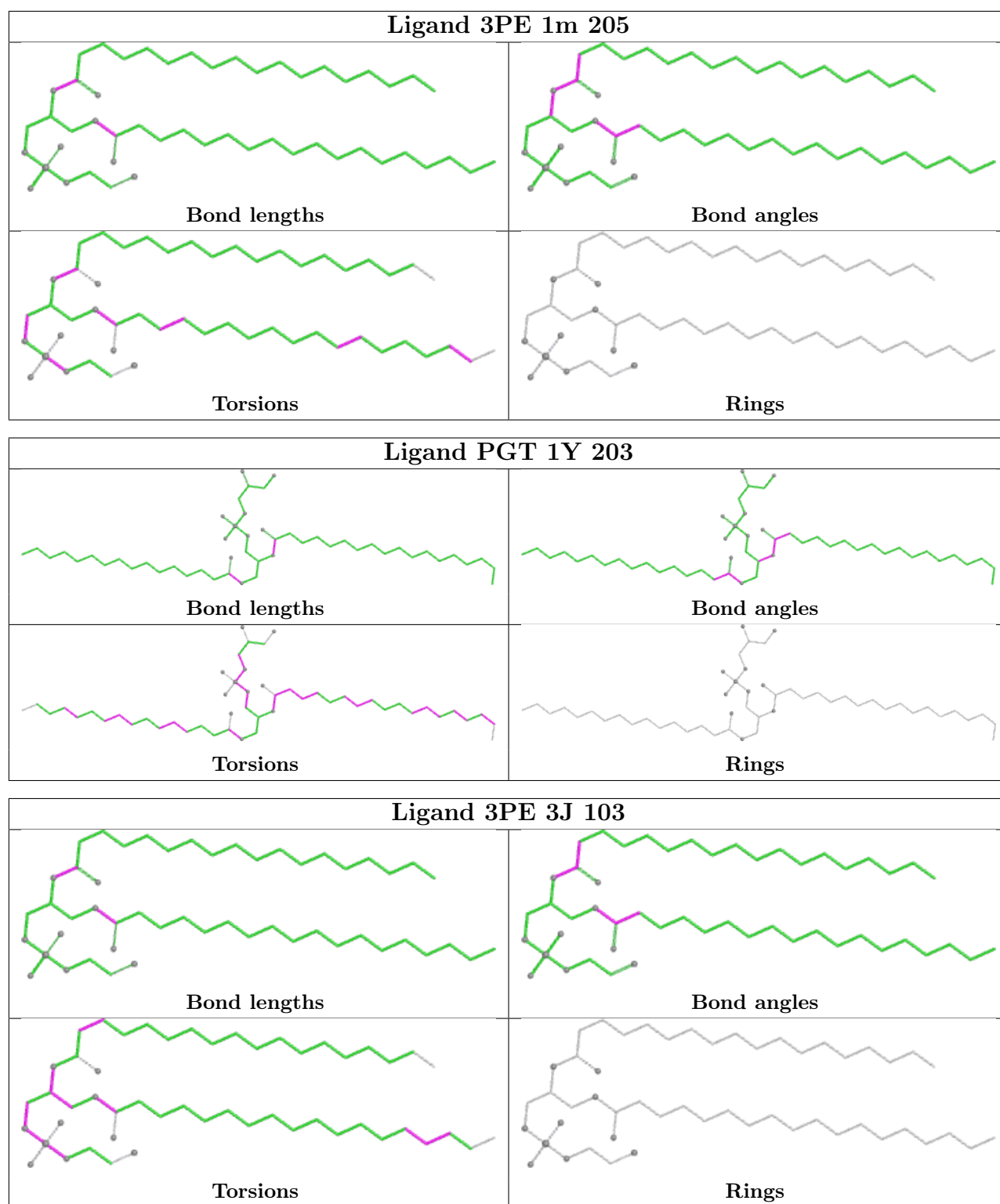


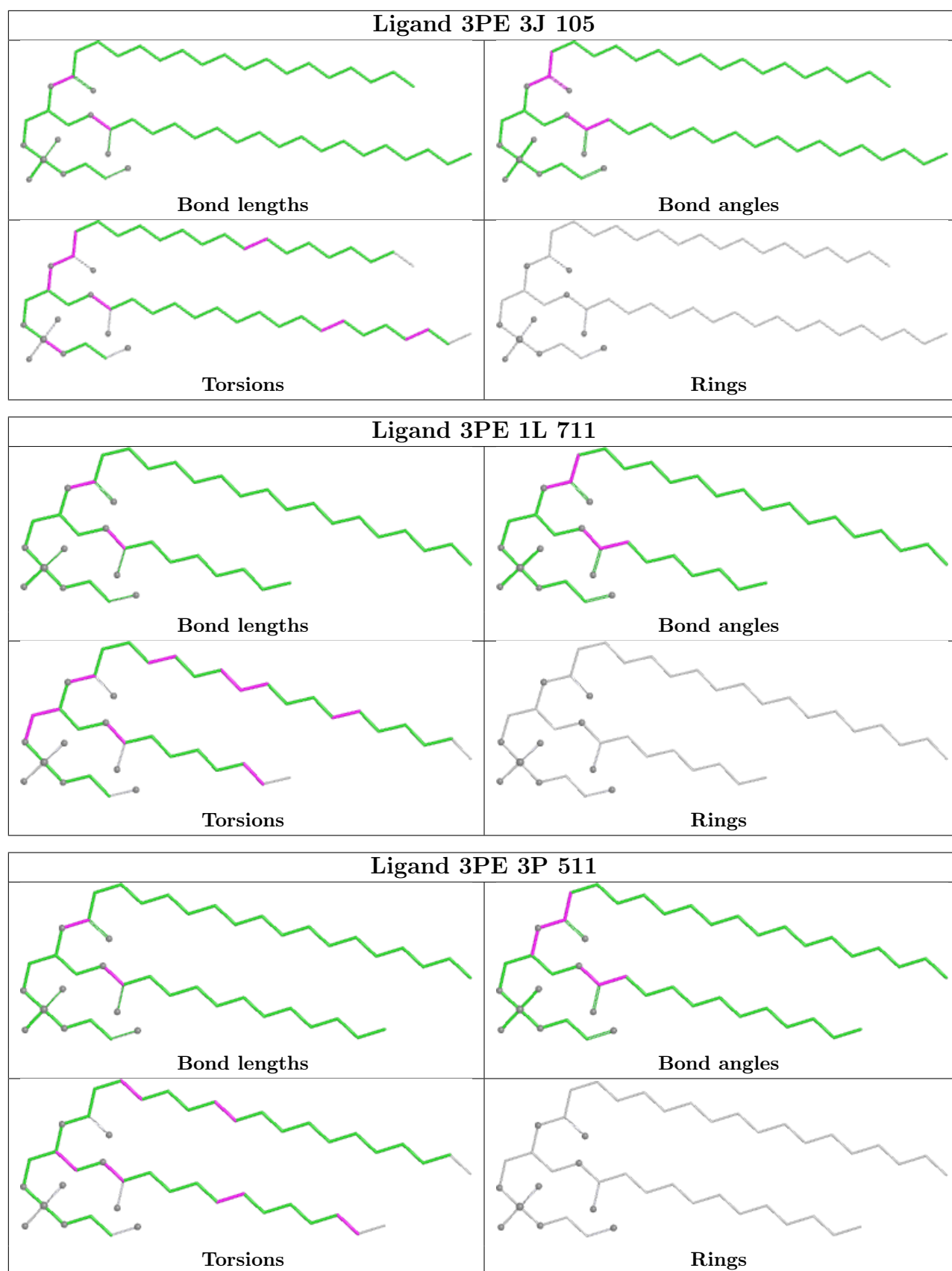


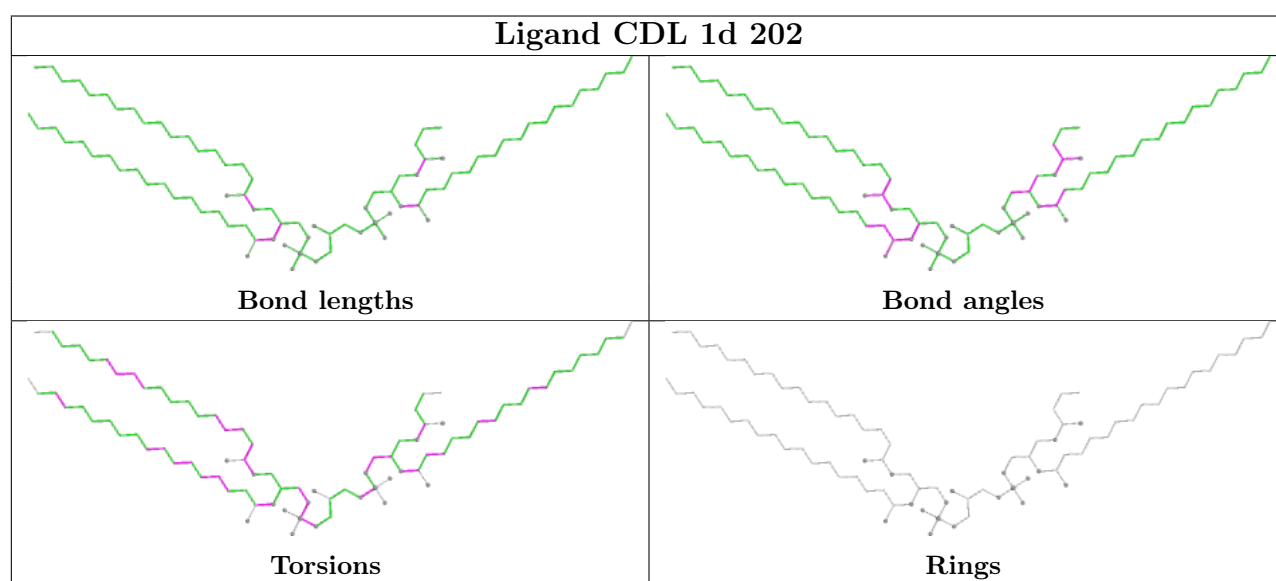
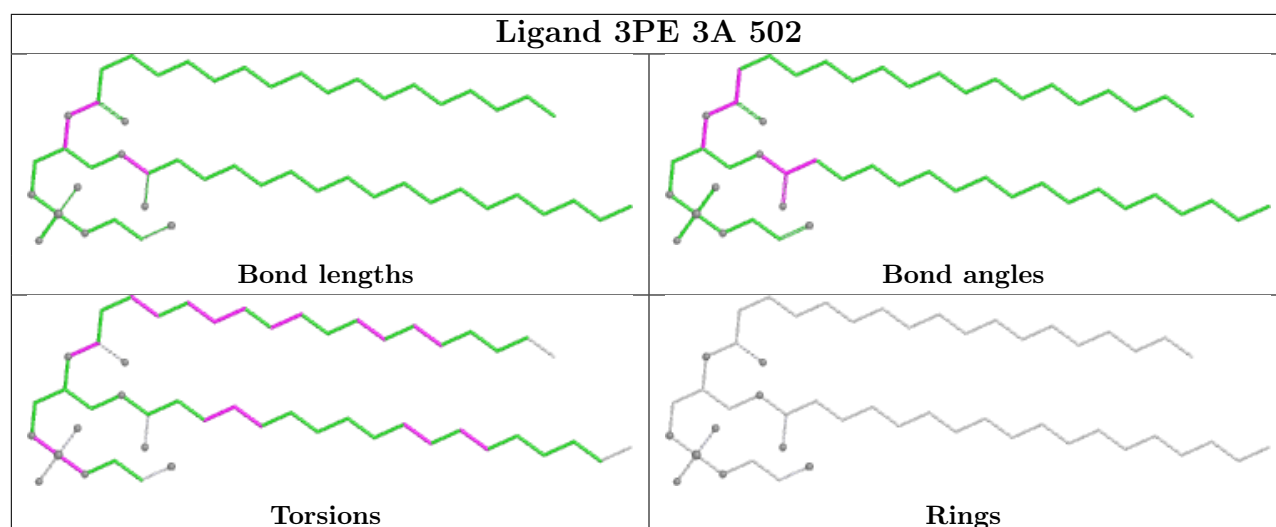


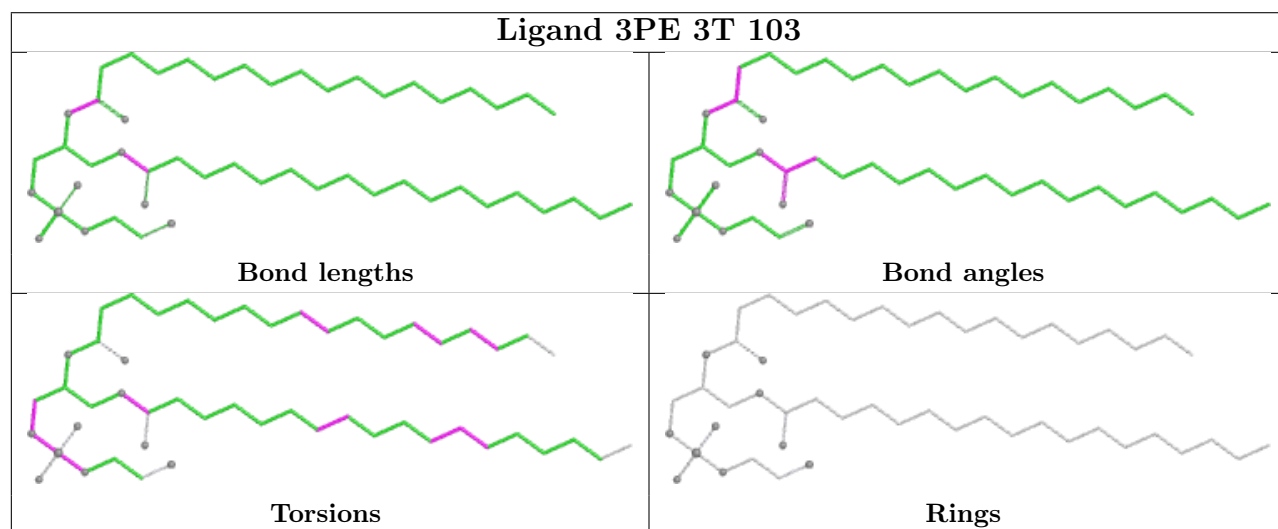
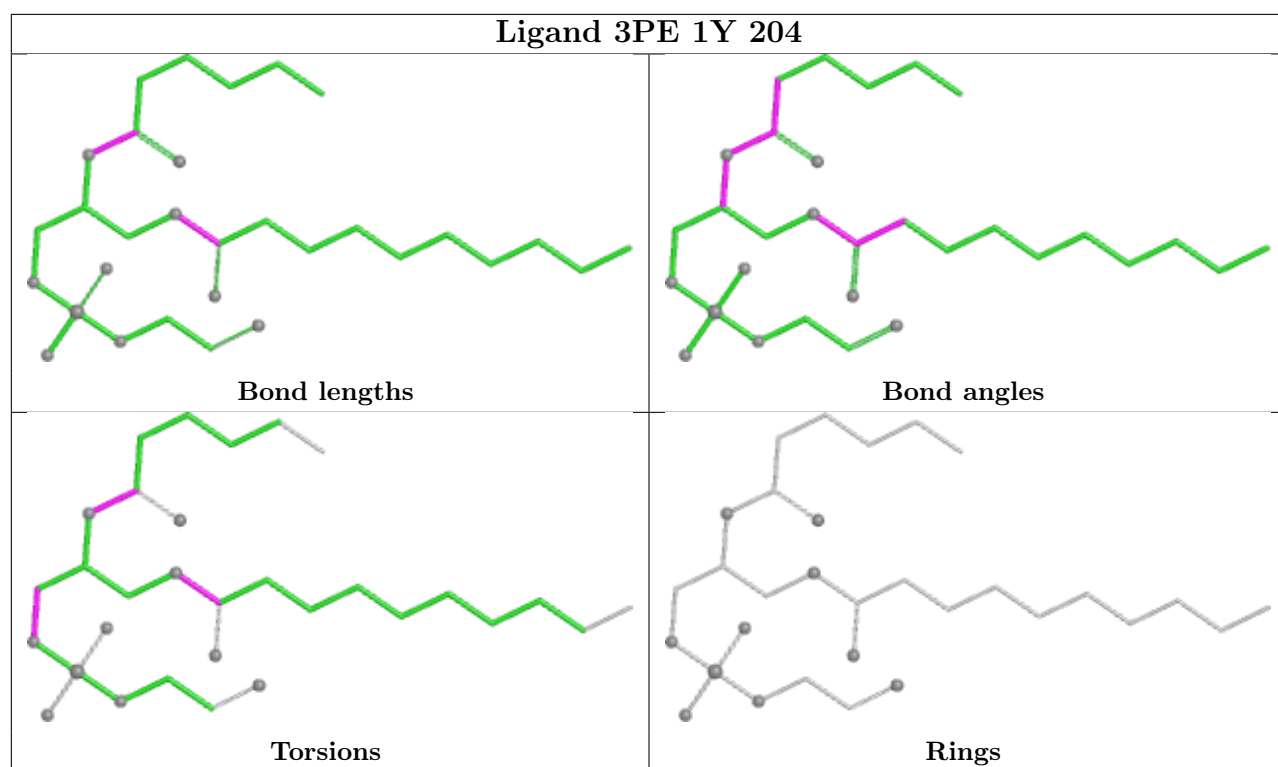


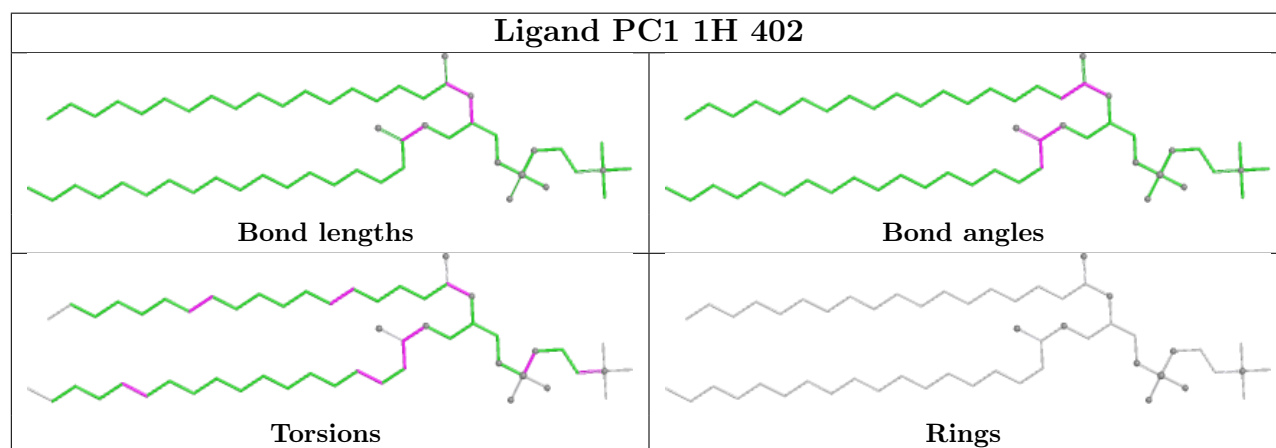
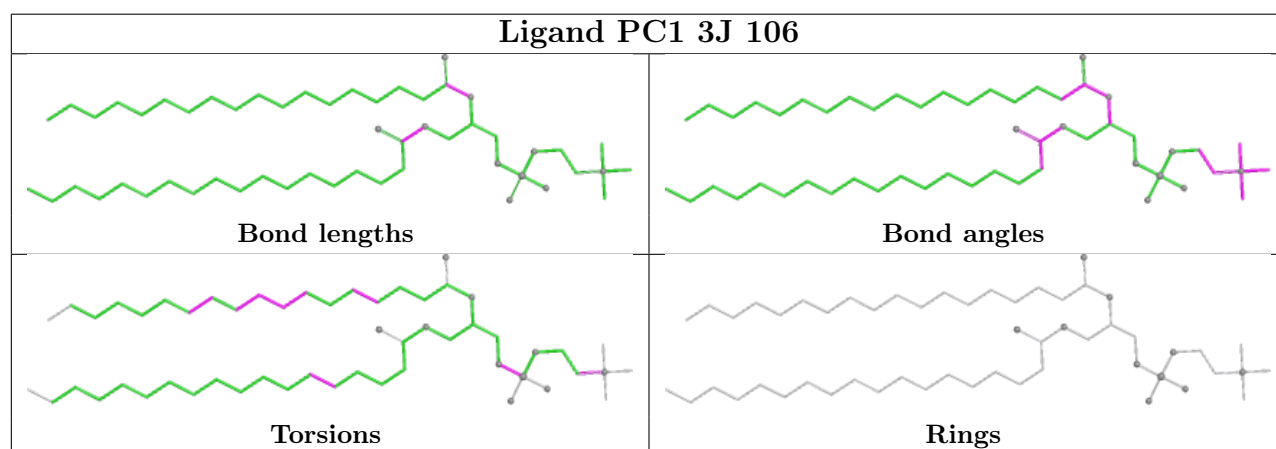
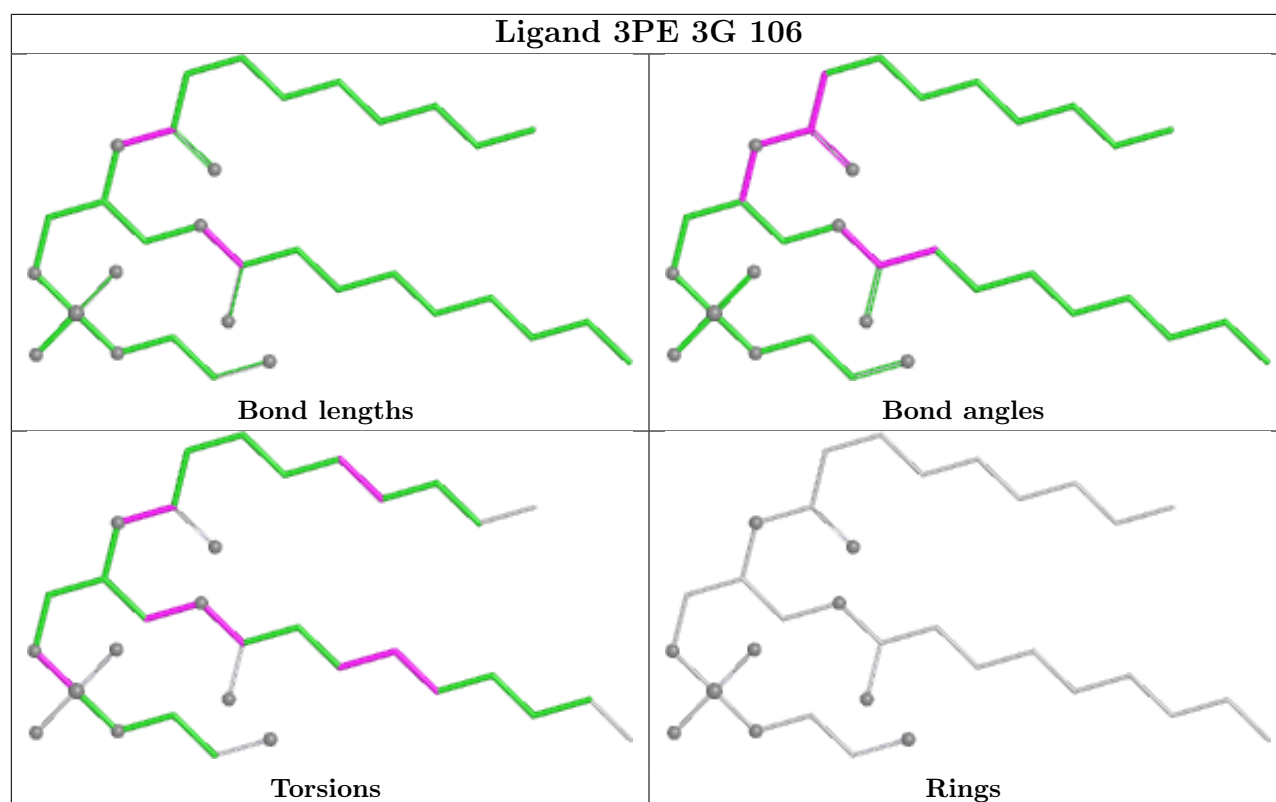


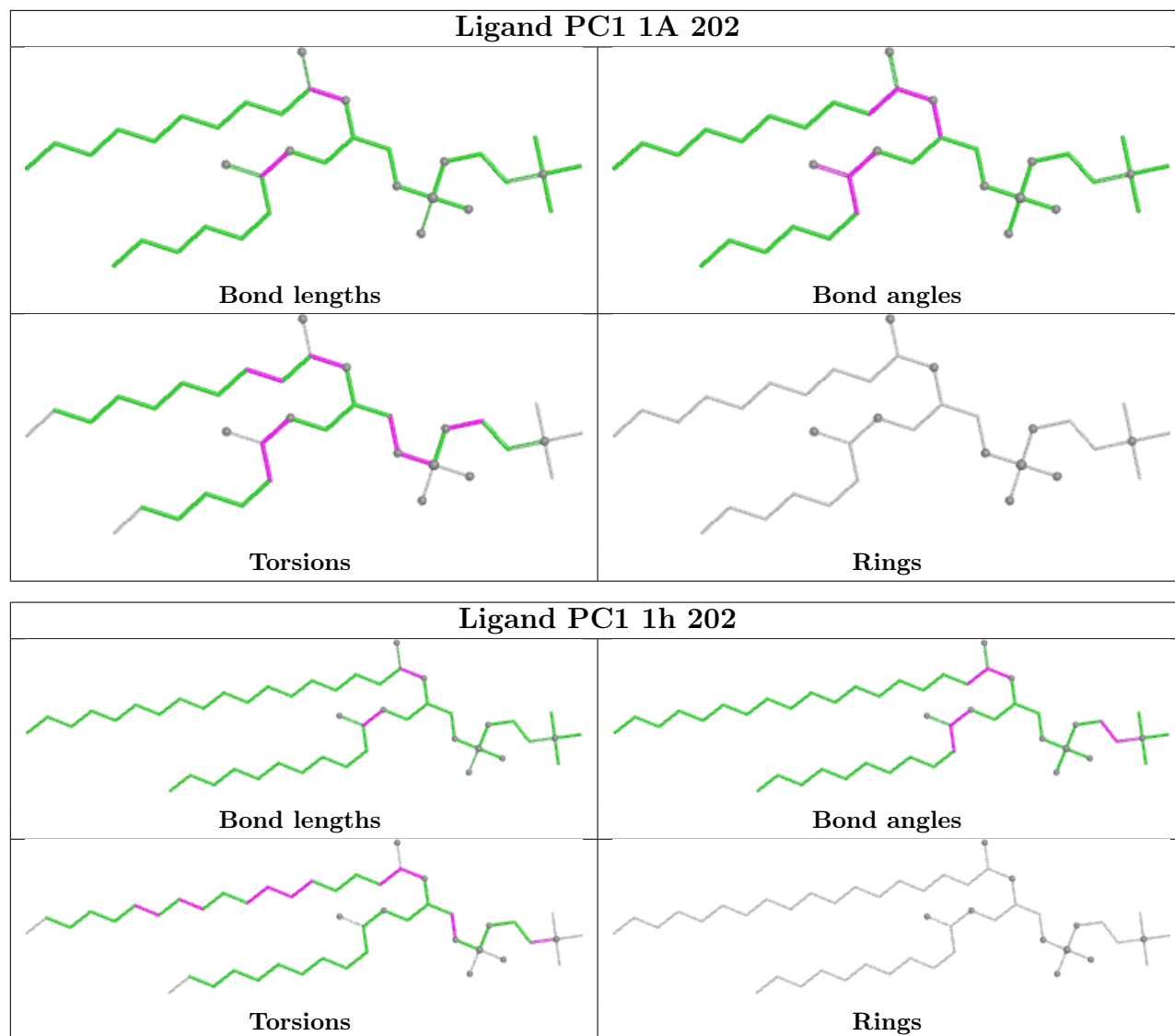


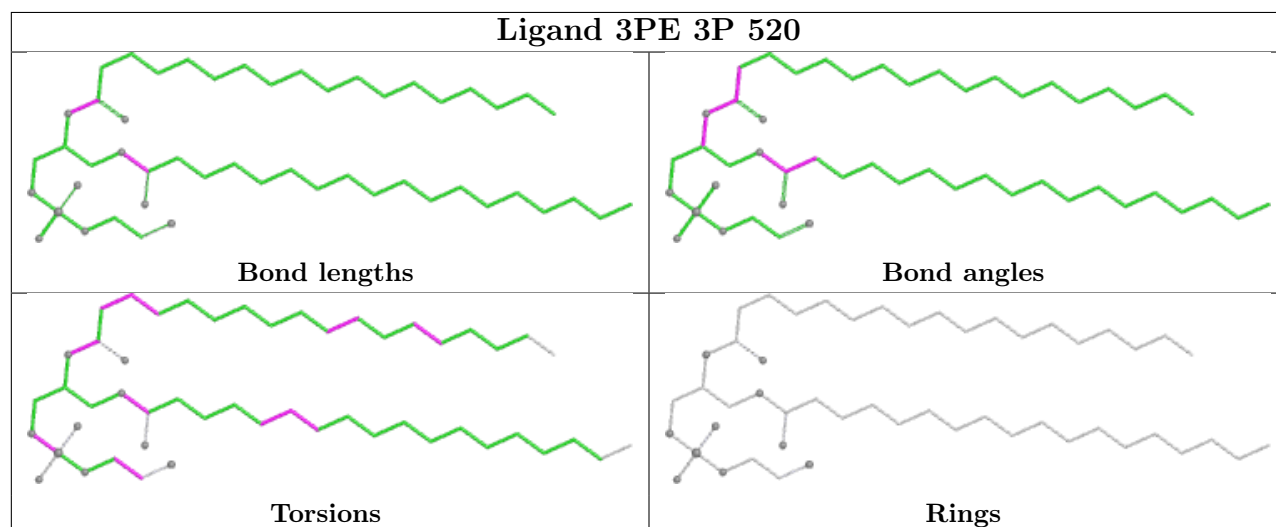
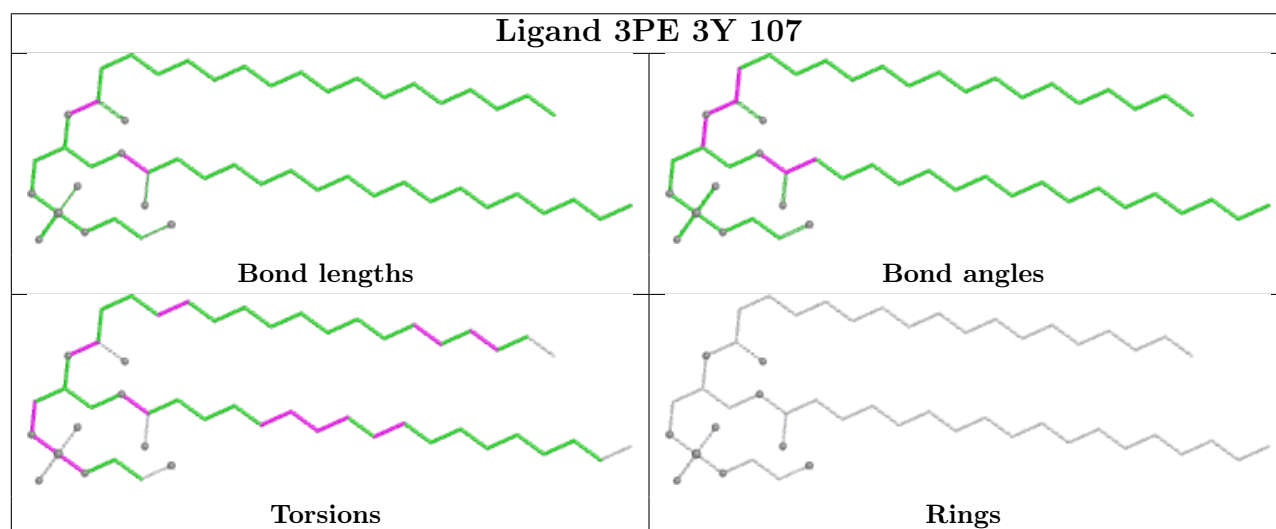
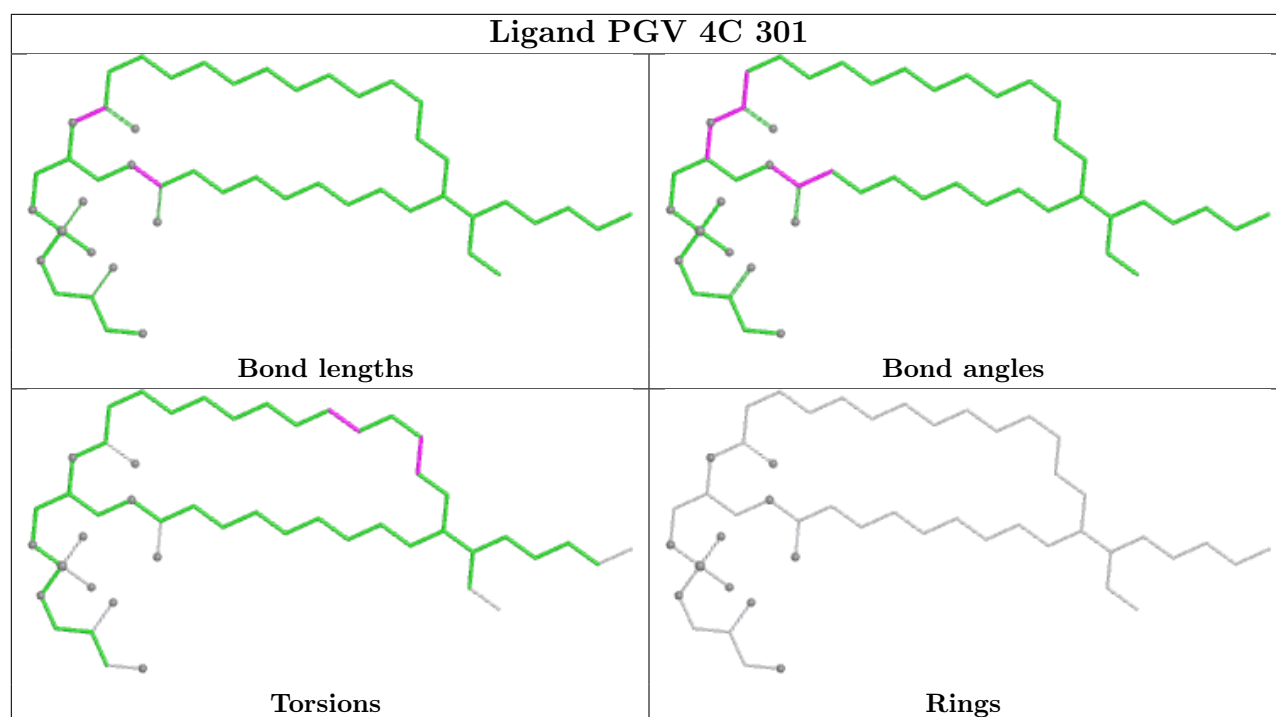


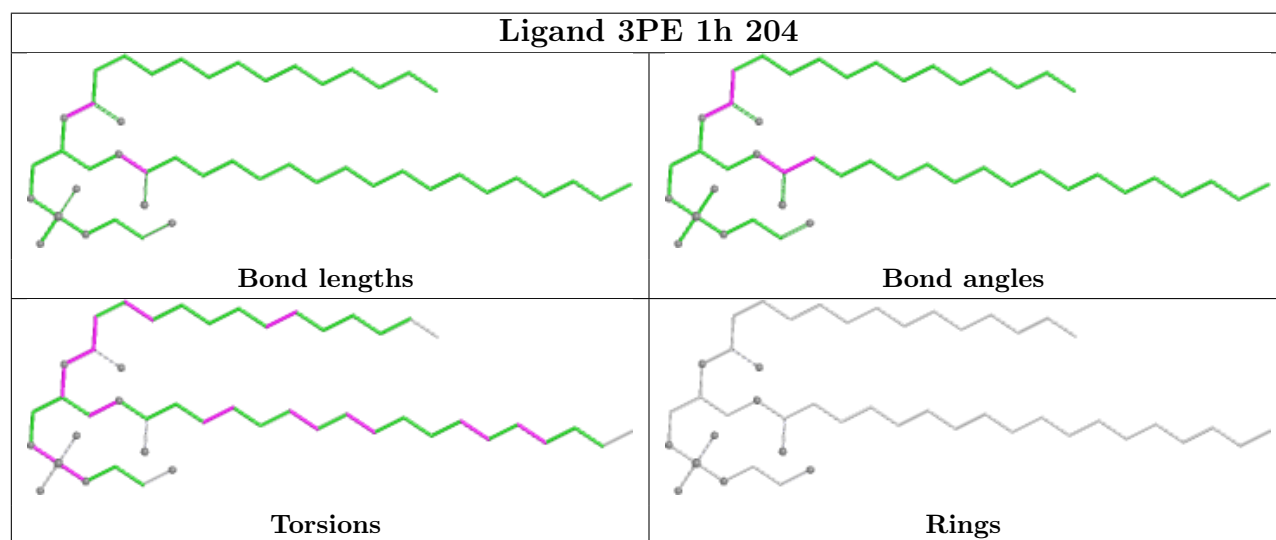
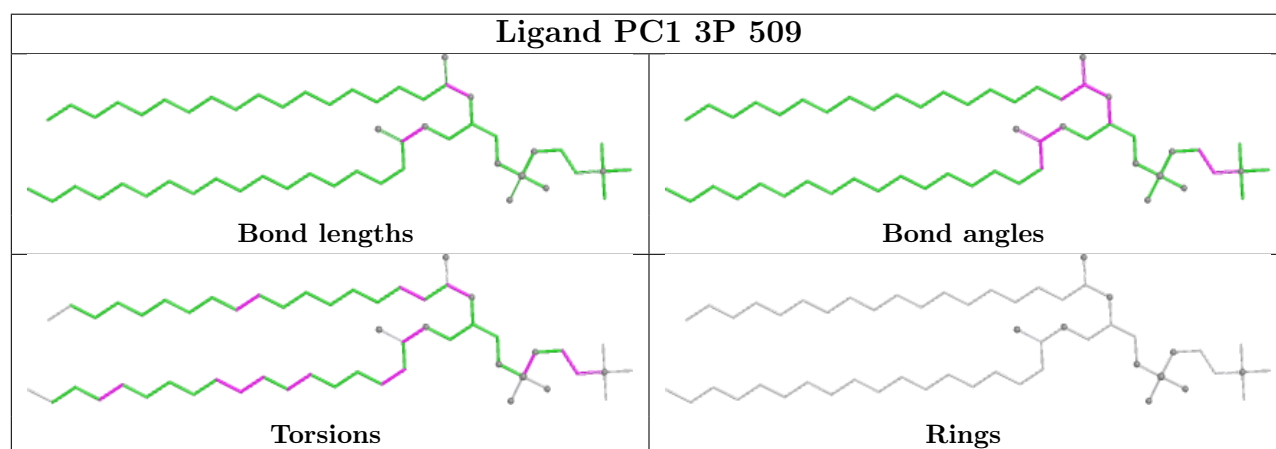
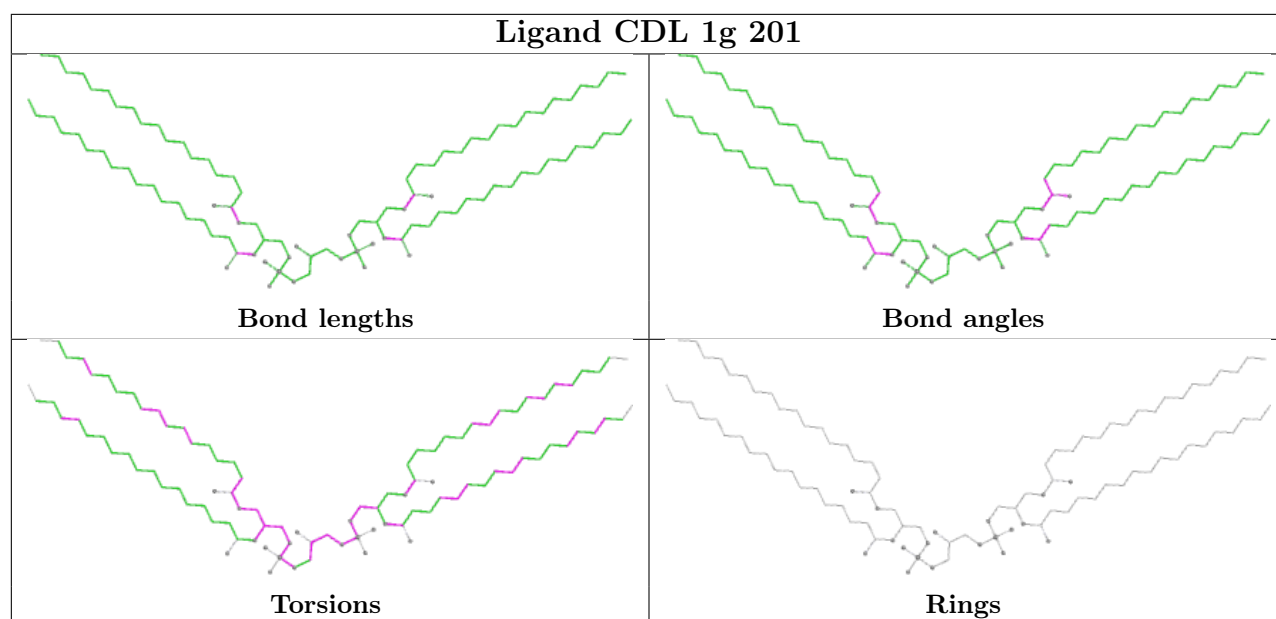


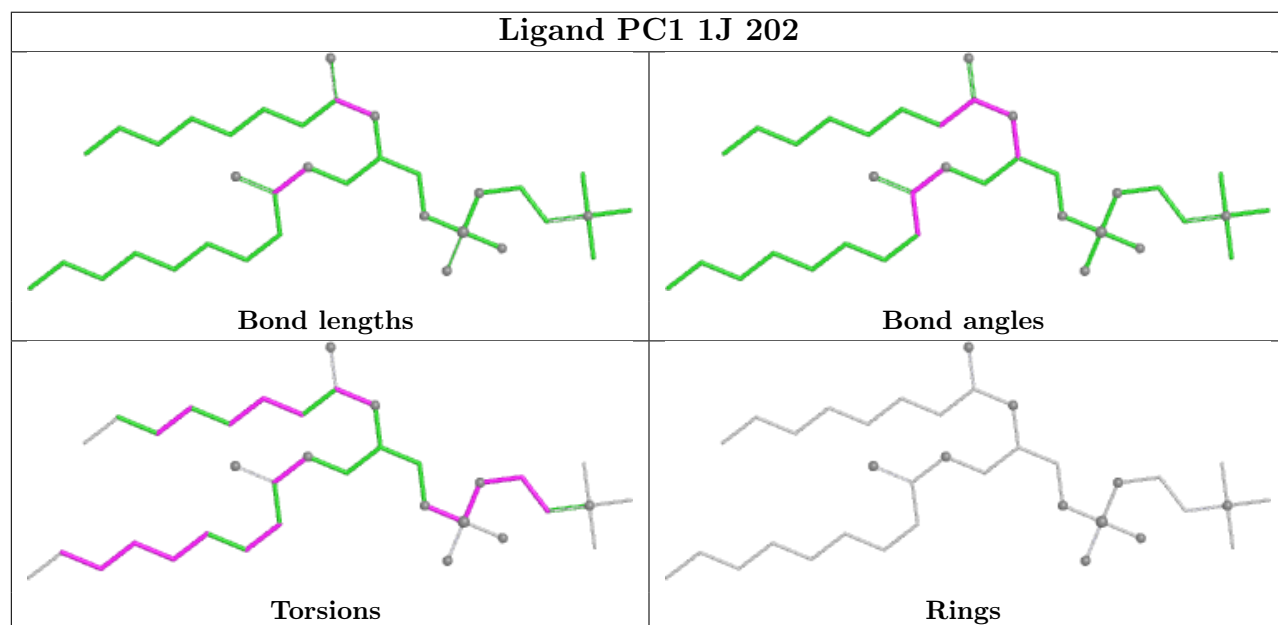
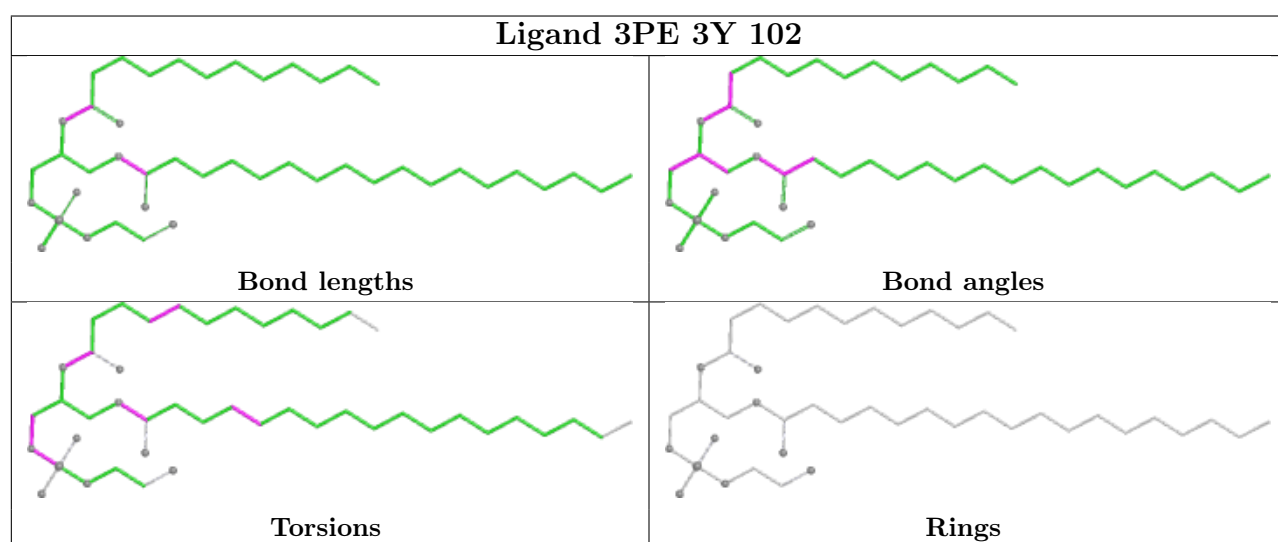
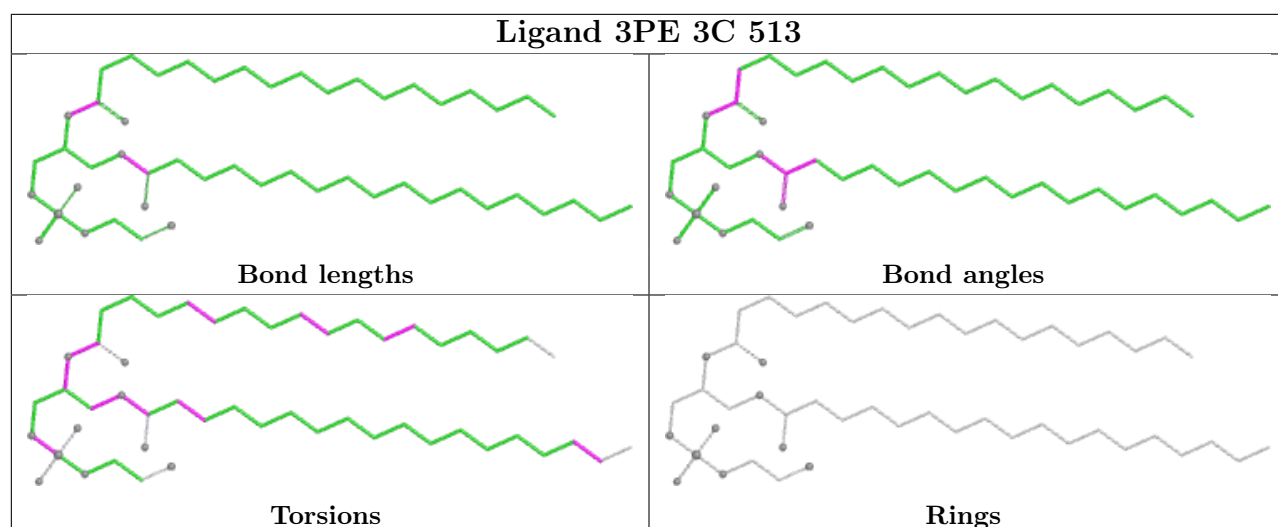


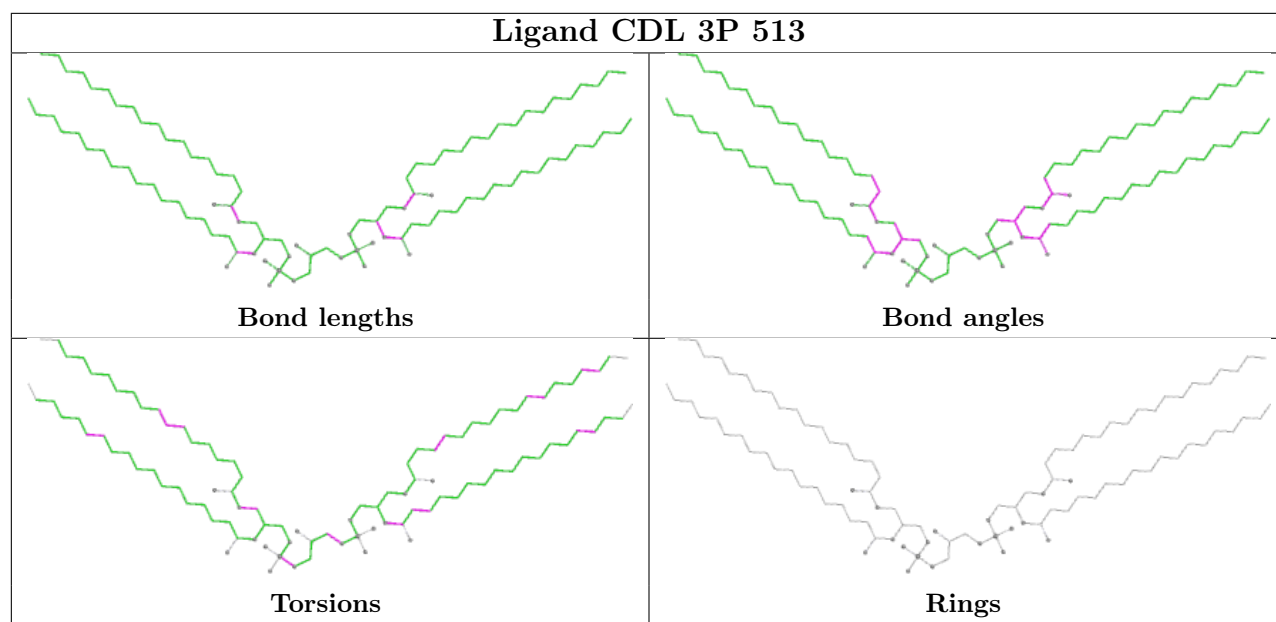
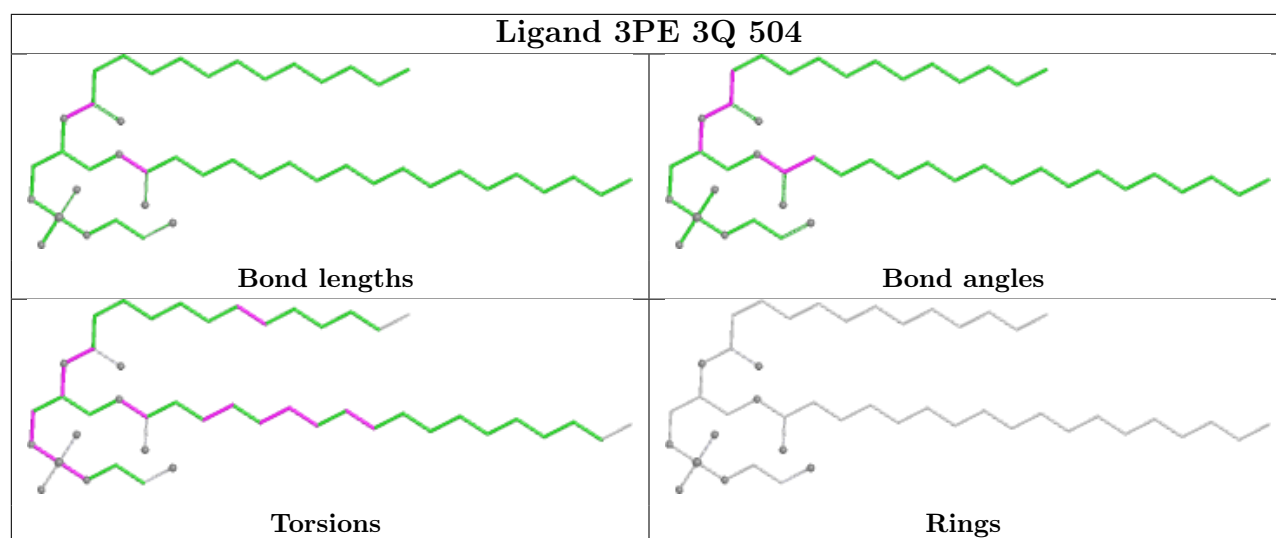


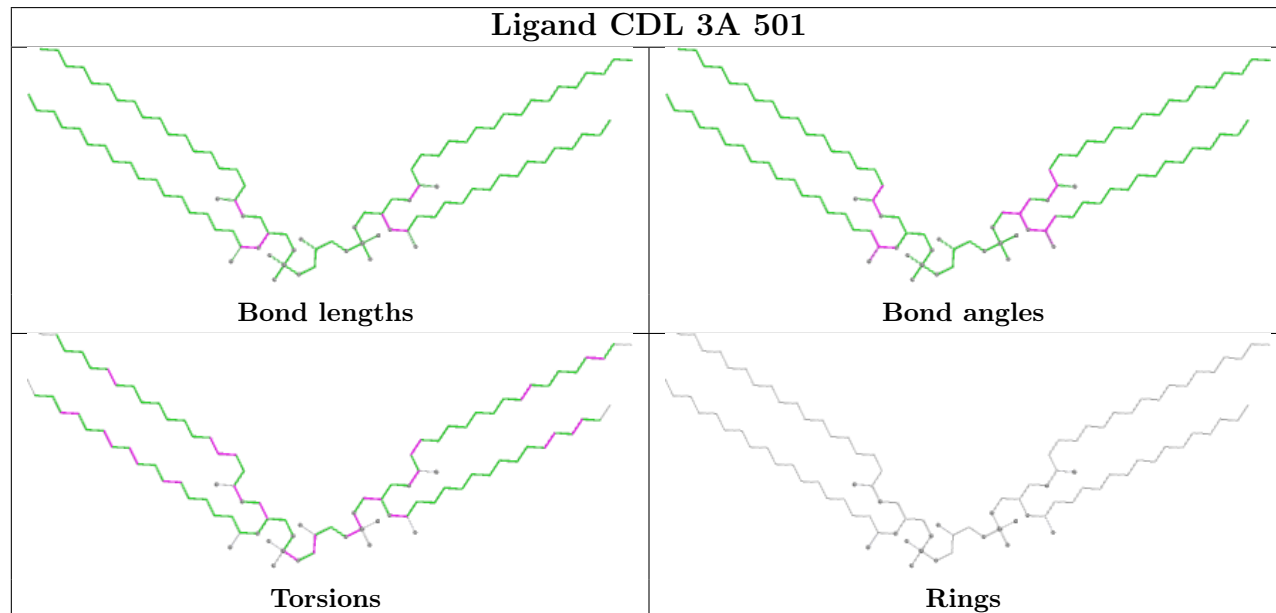
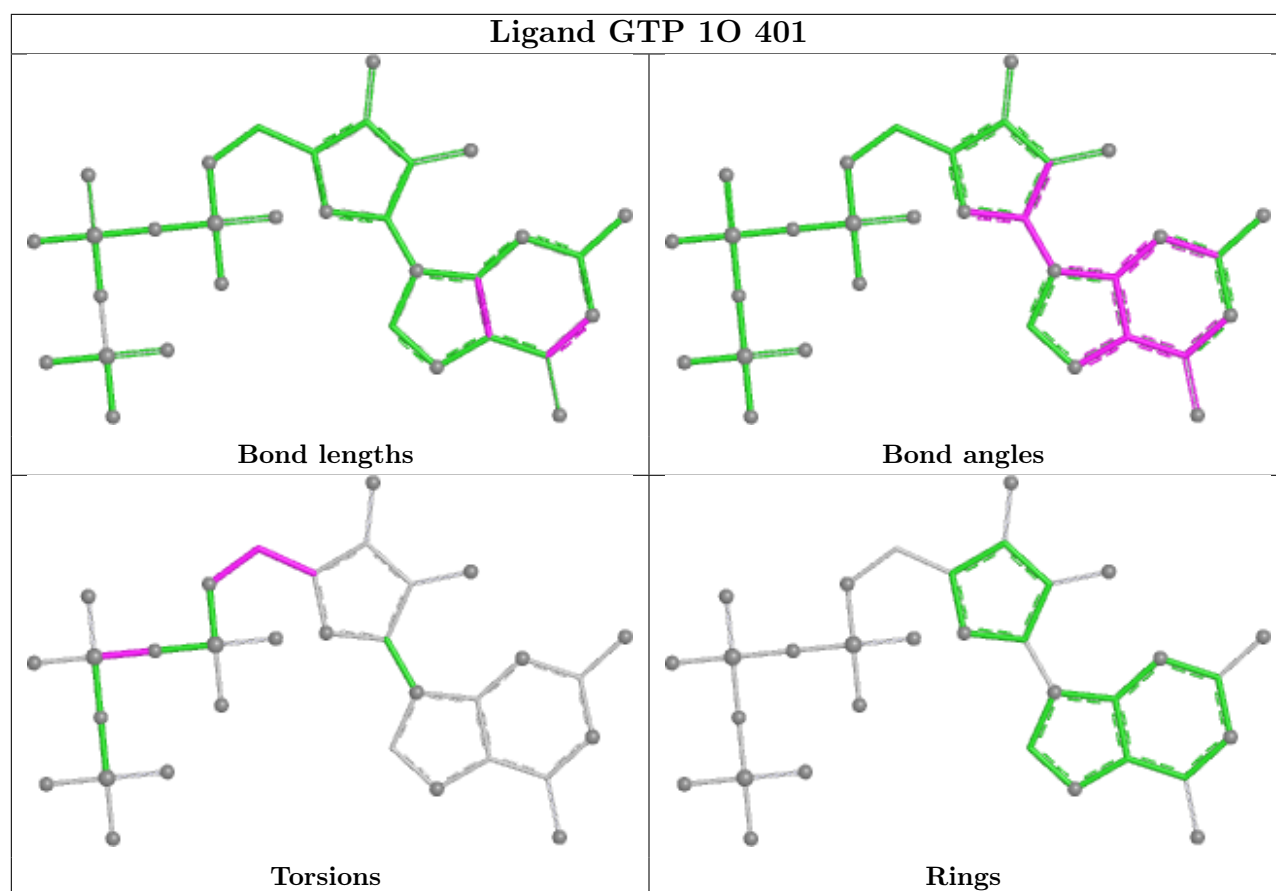


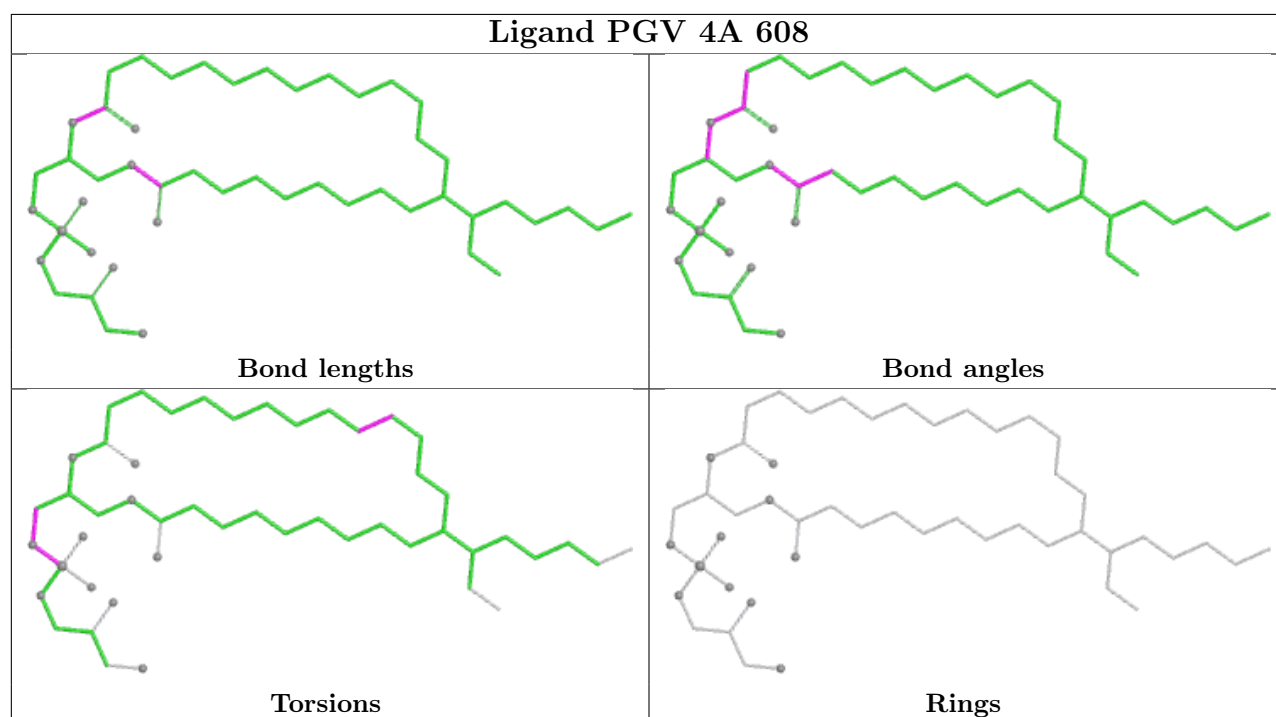
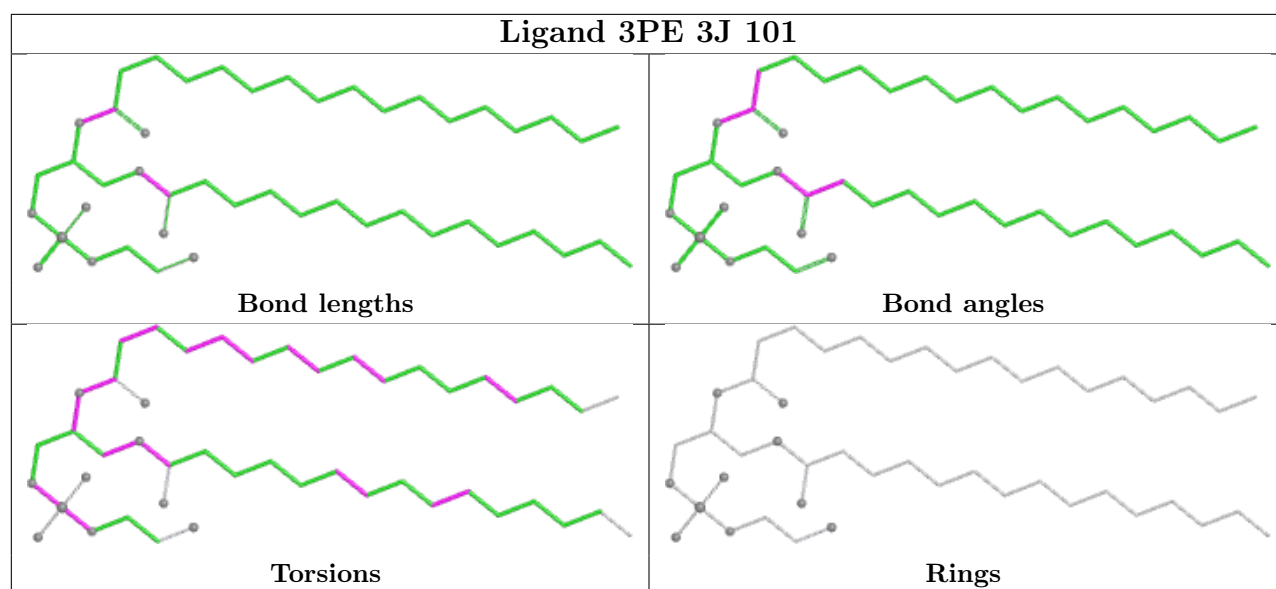




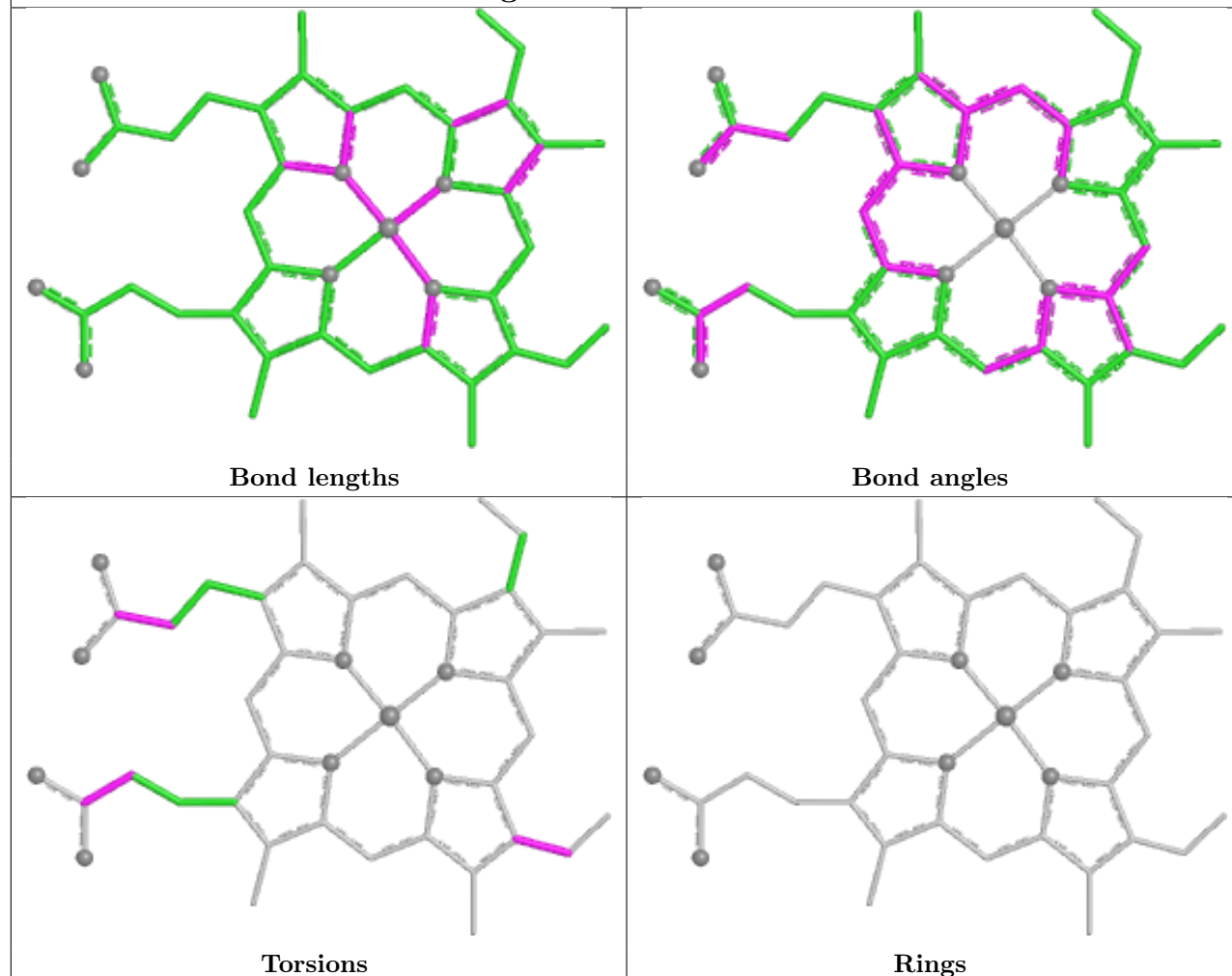




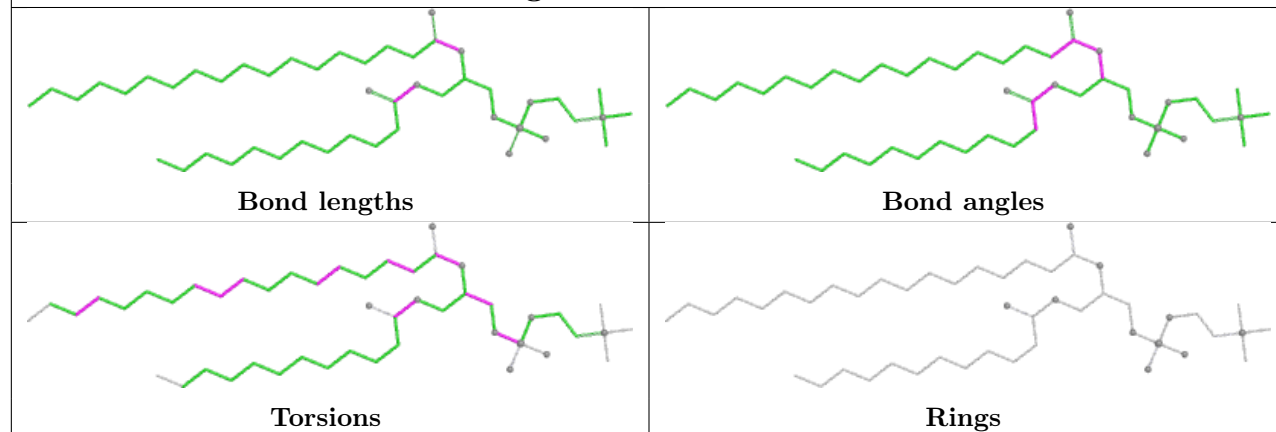


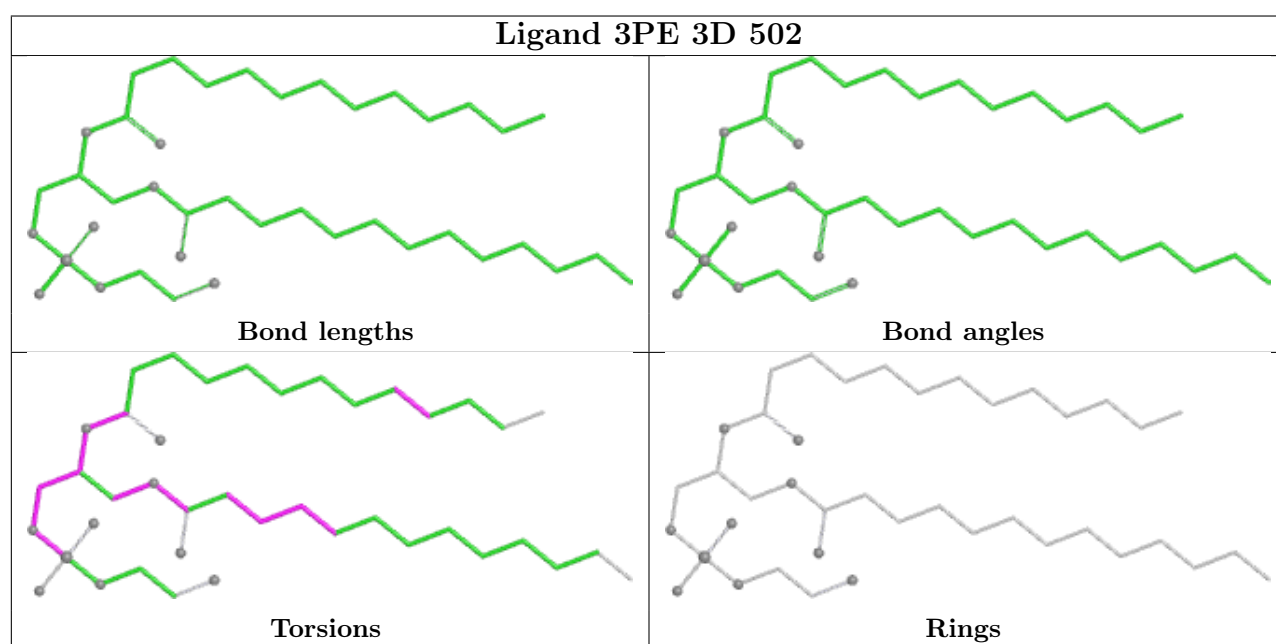
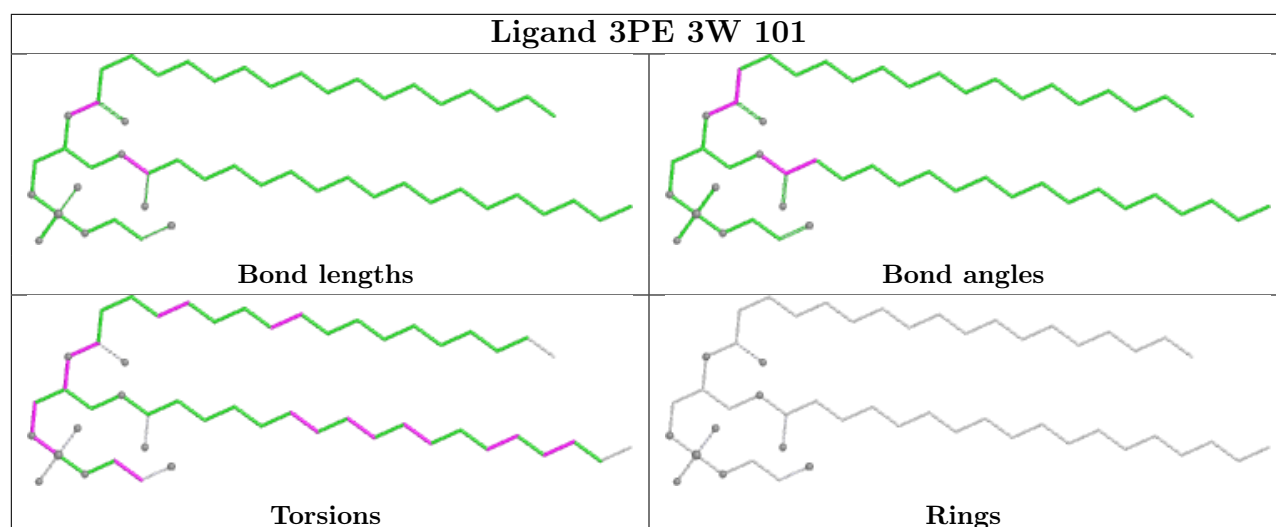


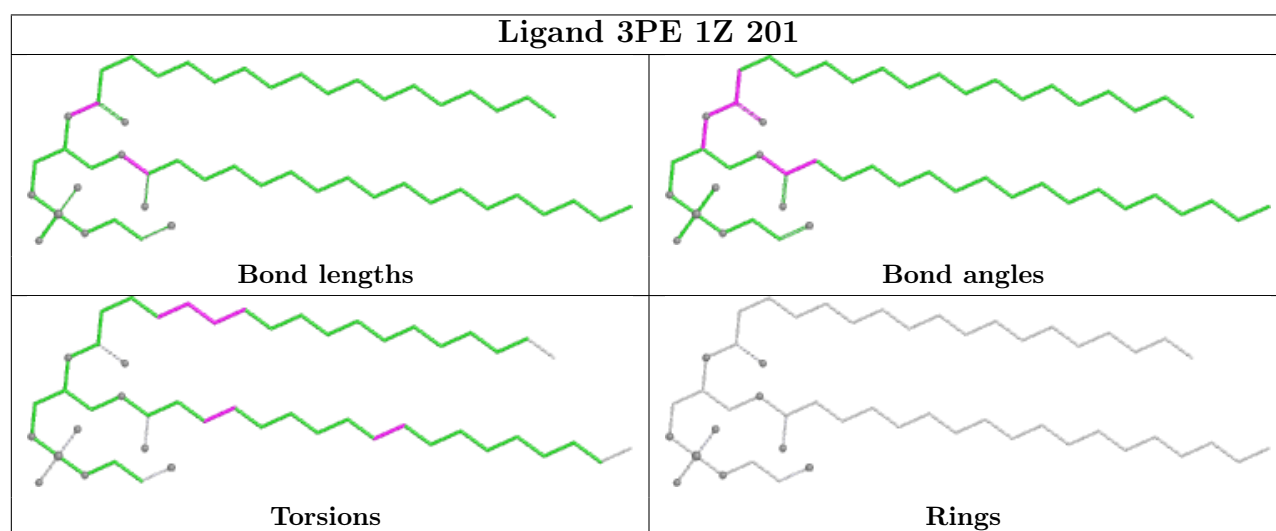
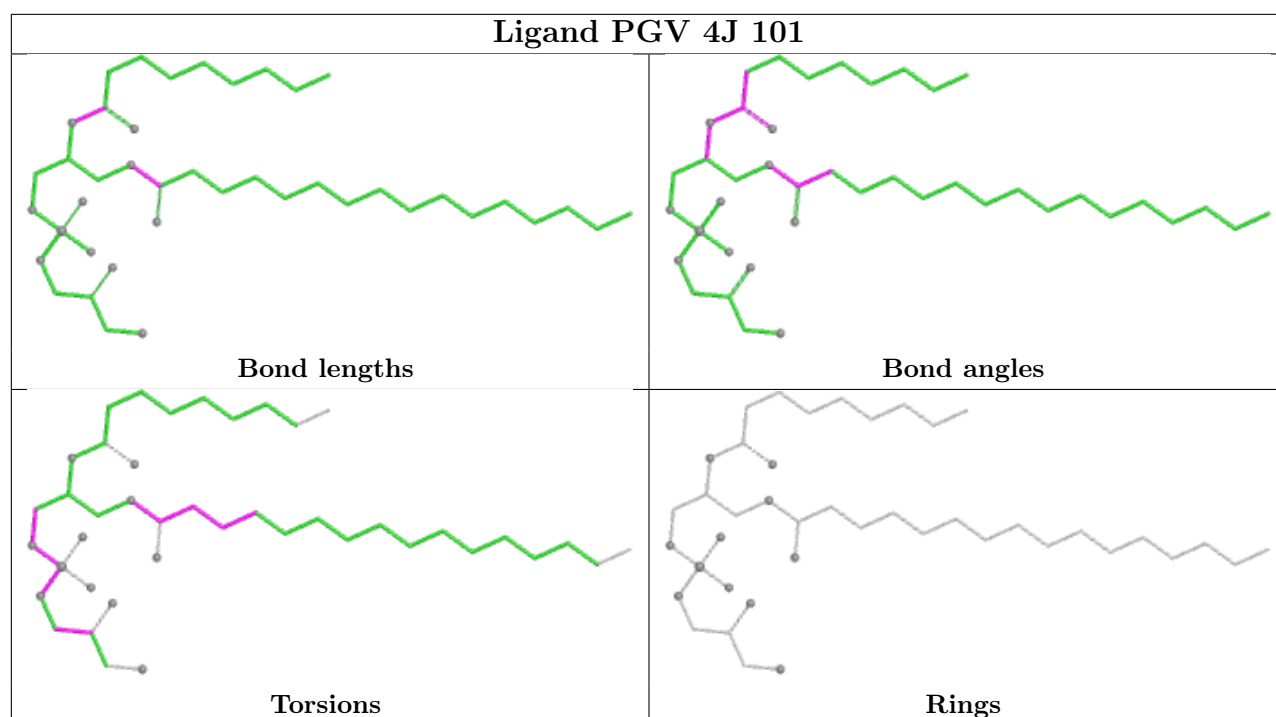
Ligand HEM 3P 501

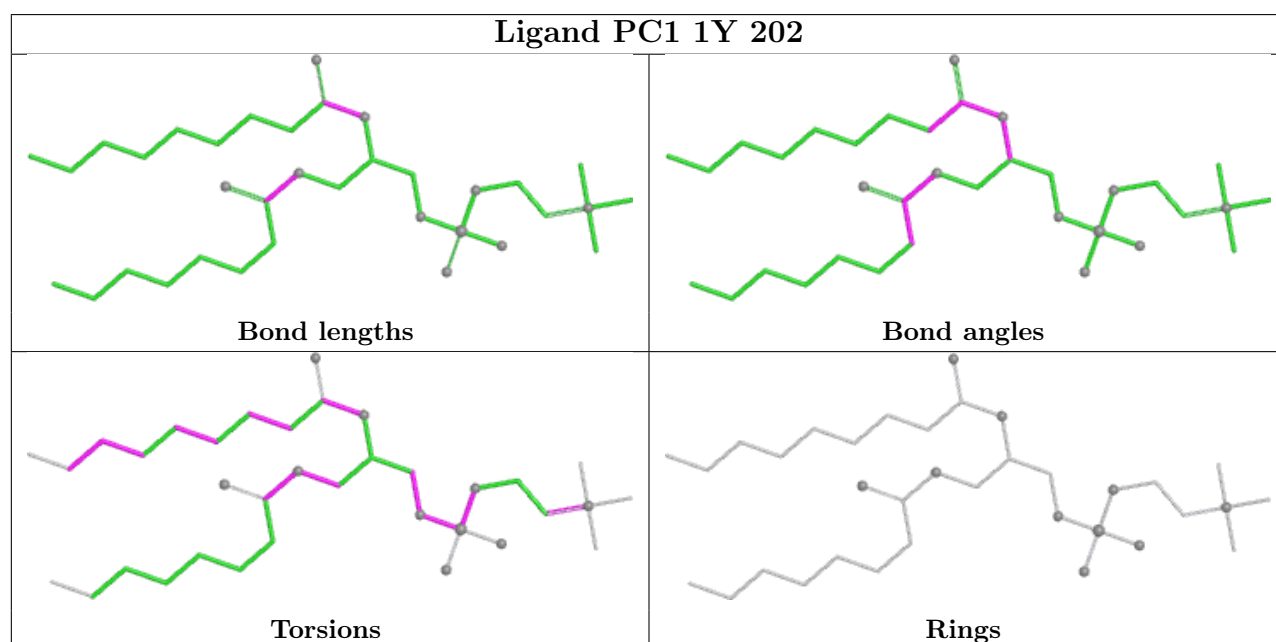
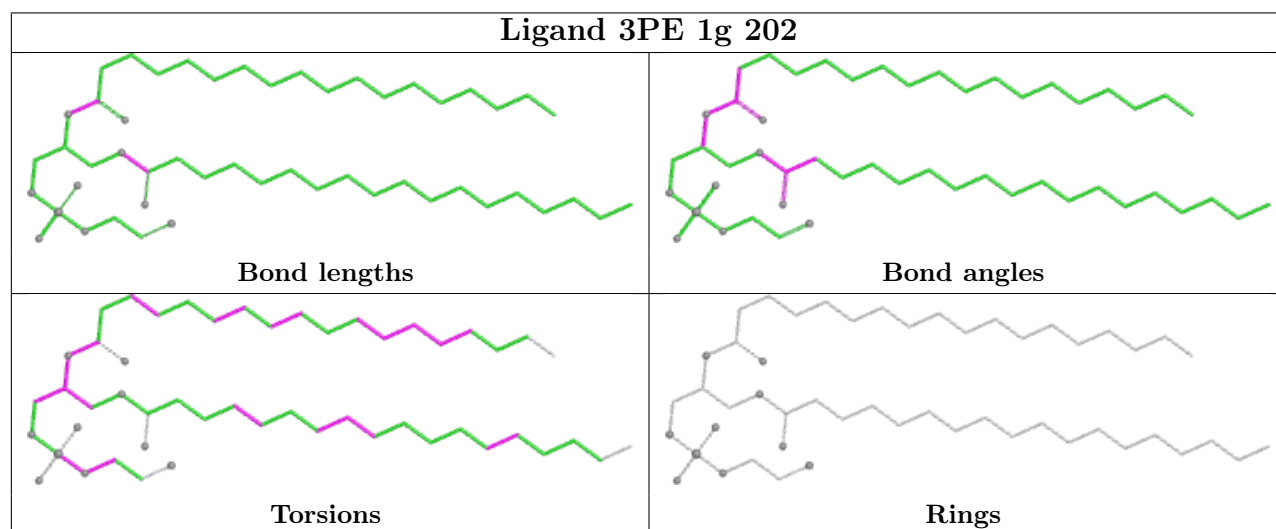
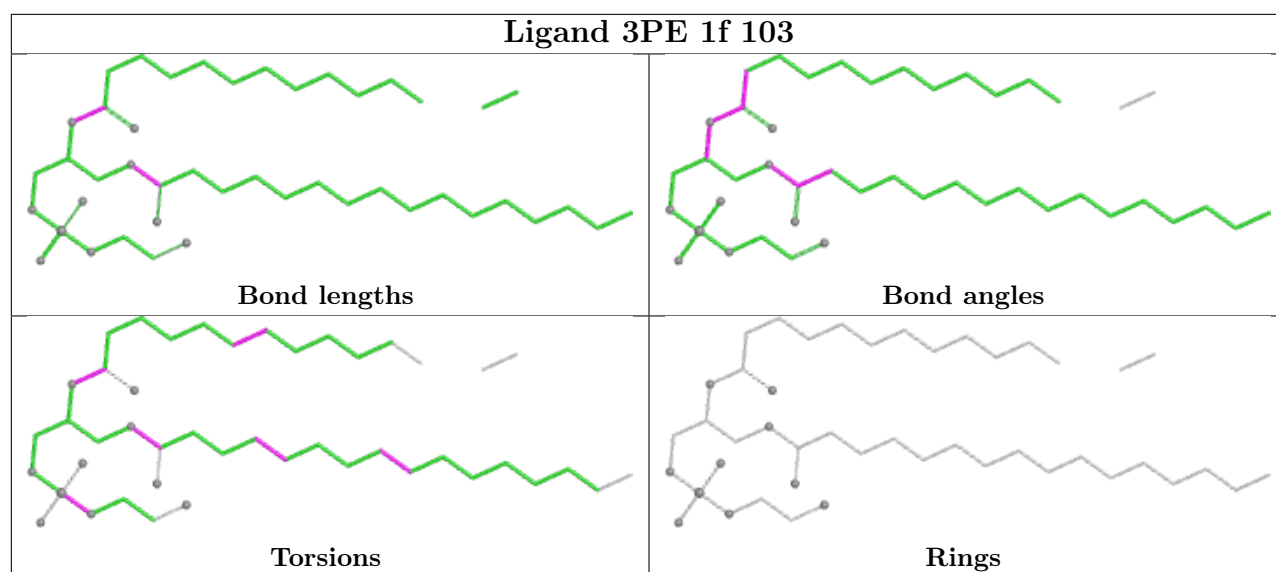


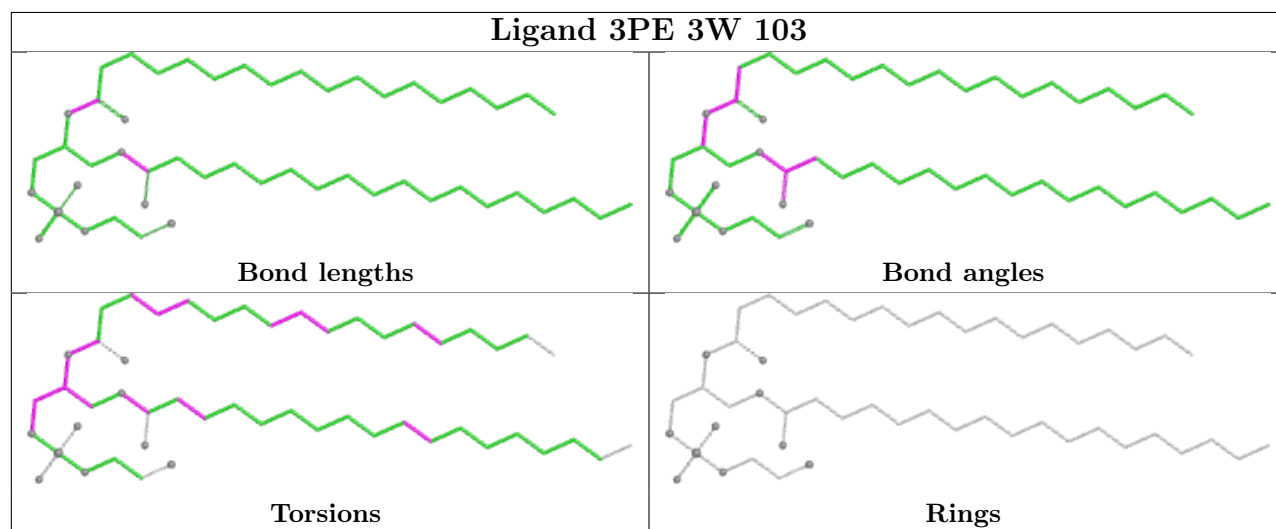
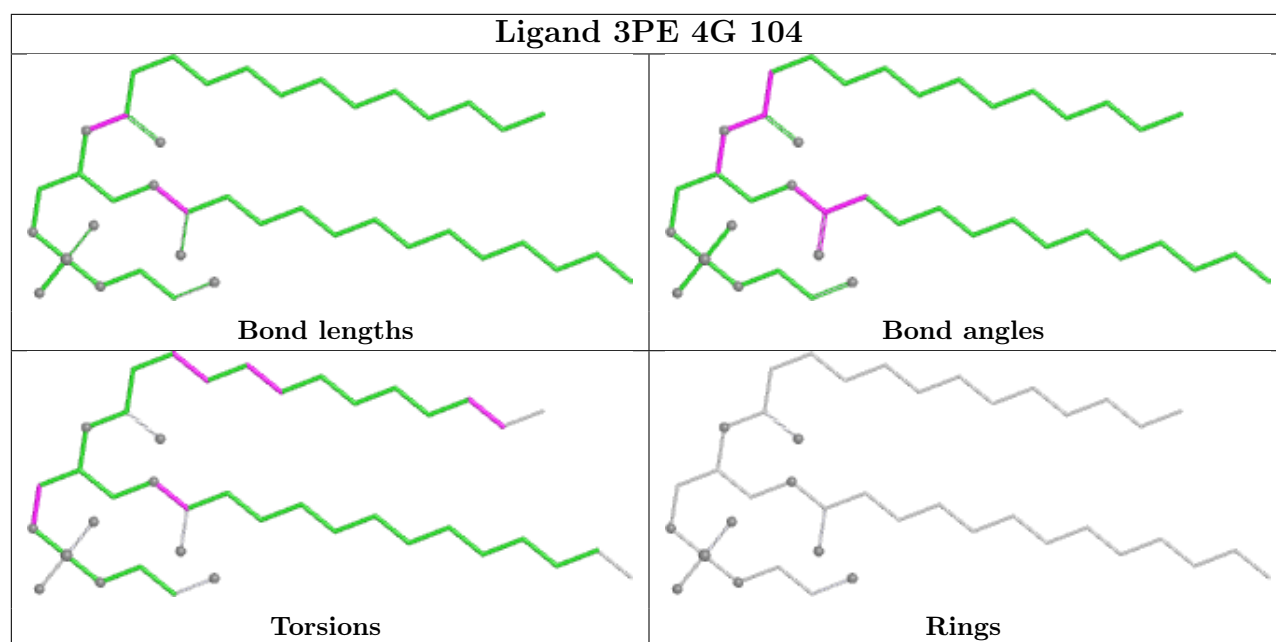
Ligand PC1 1H 403

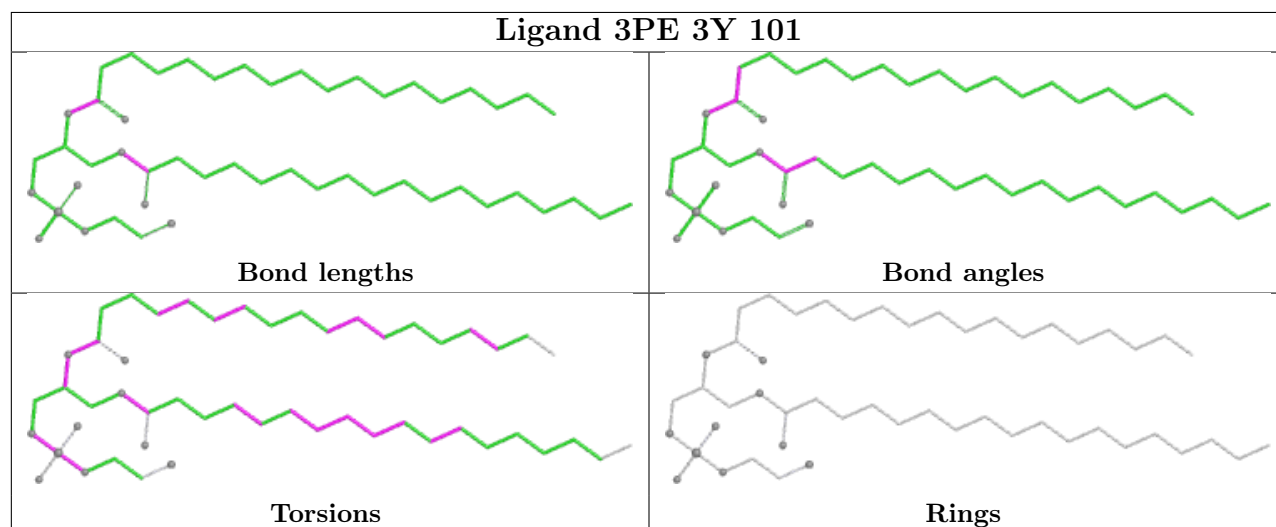
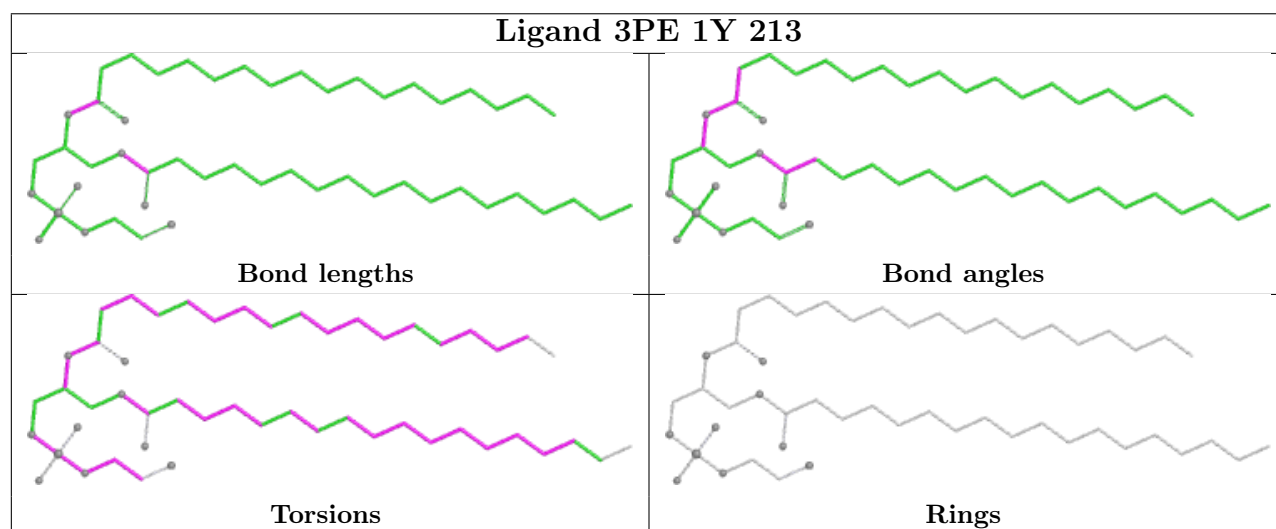
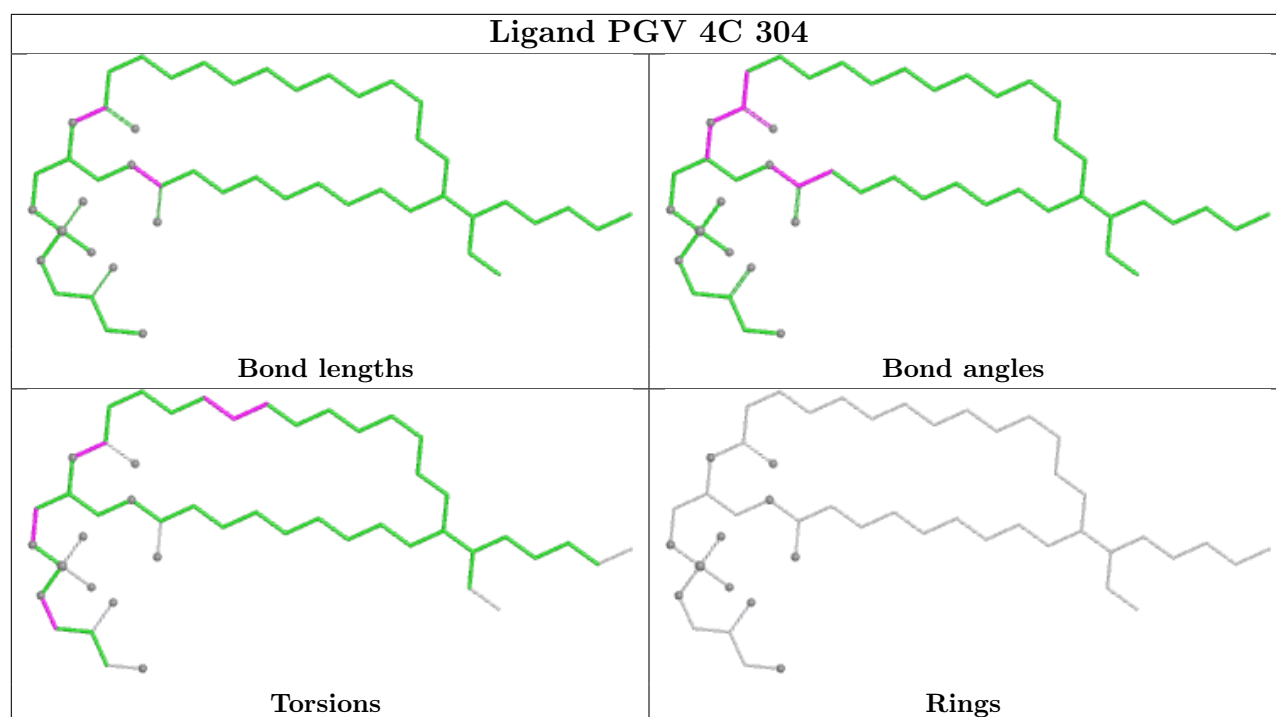


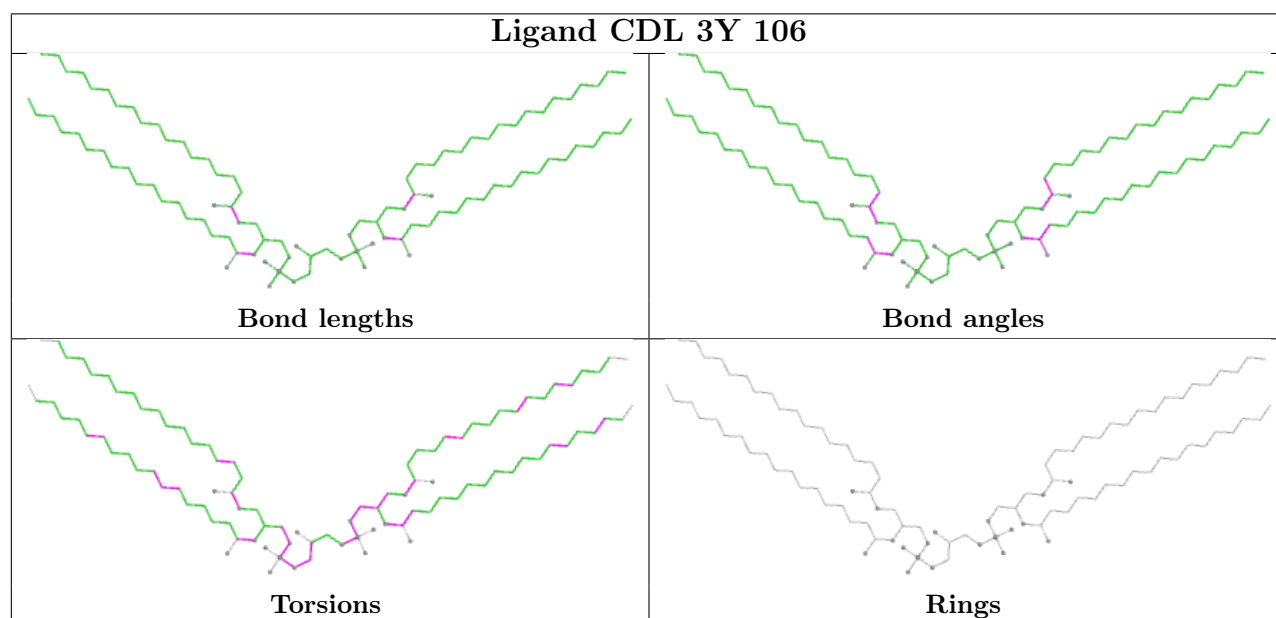
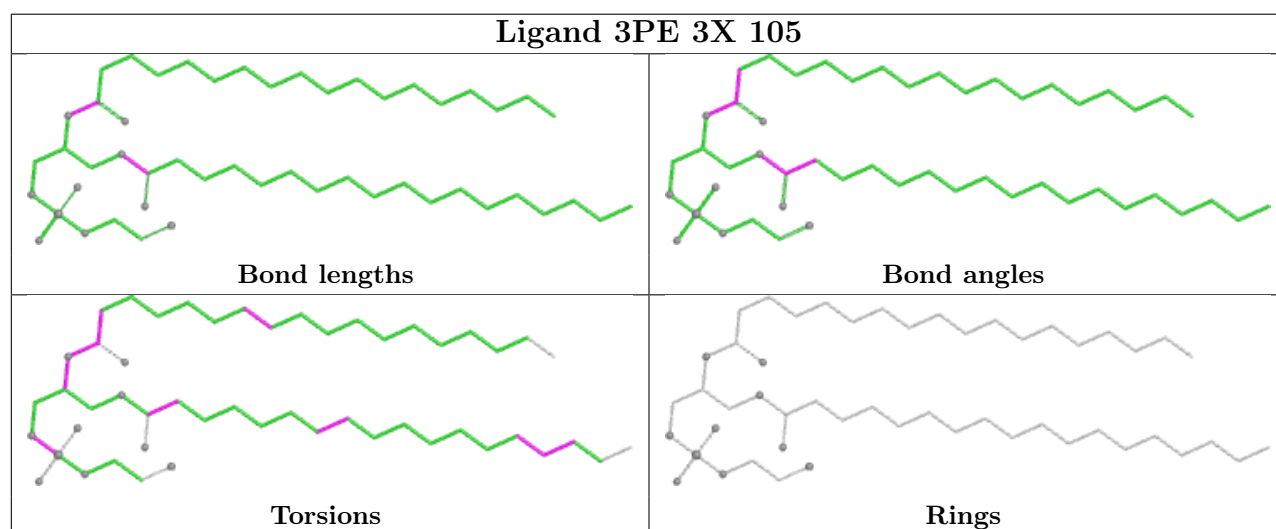
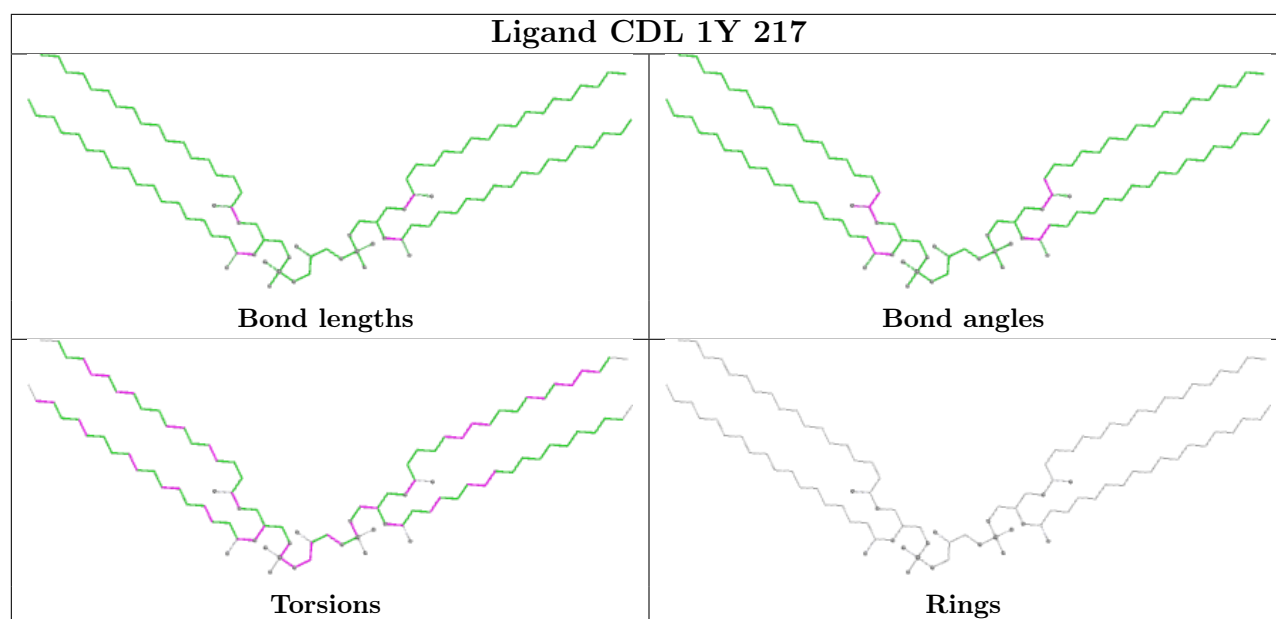


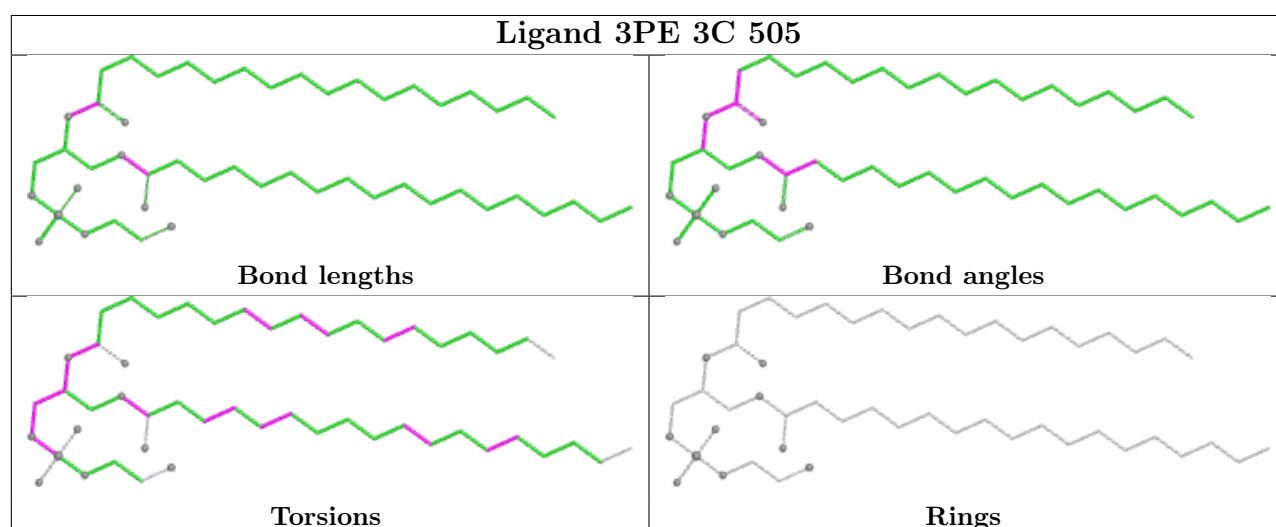
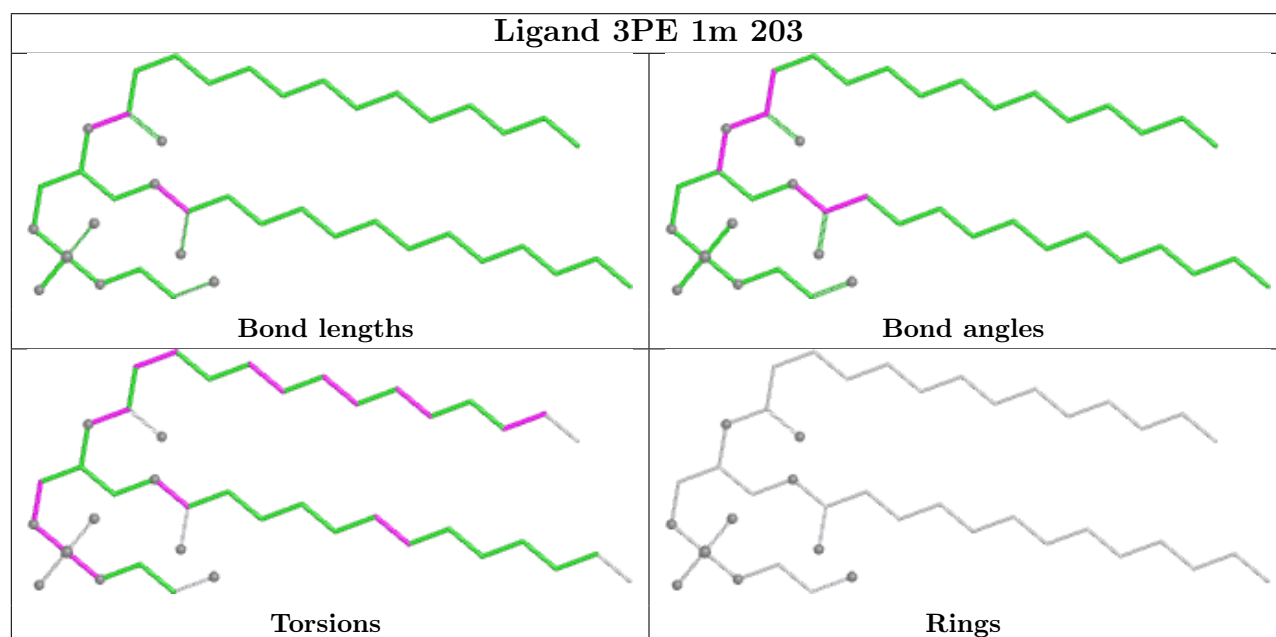
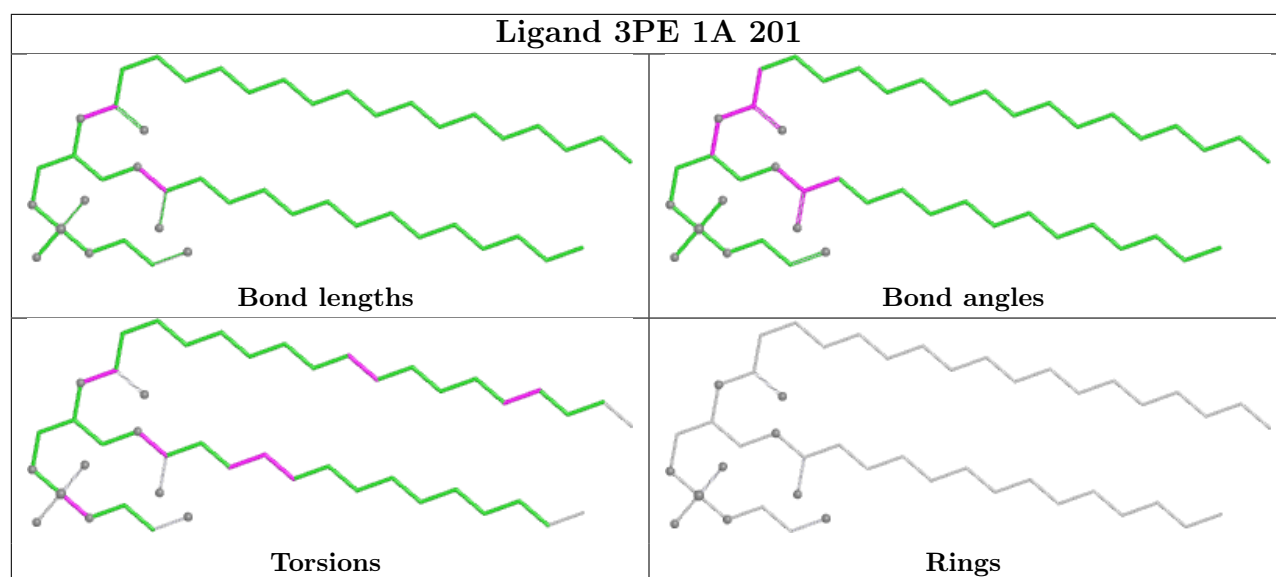


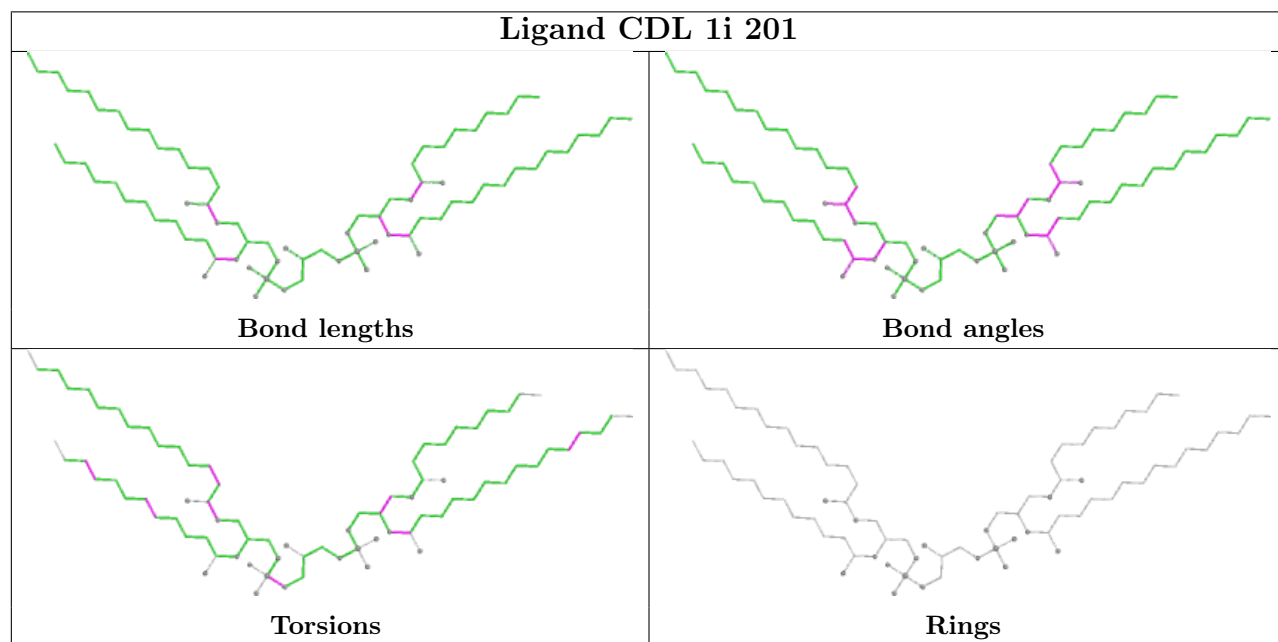
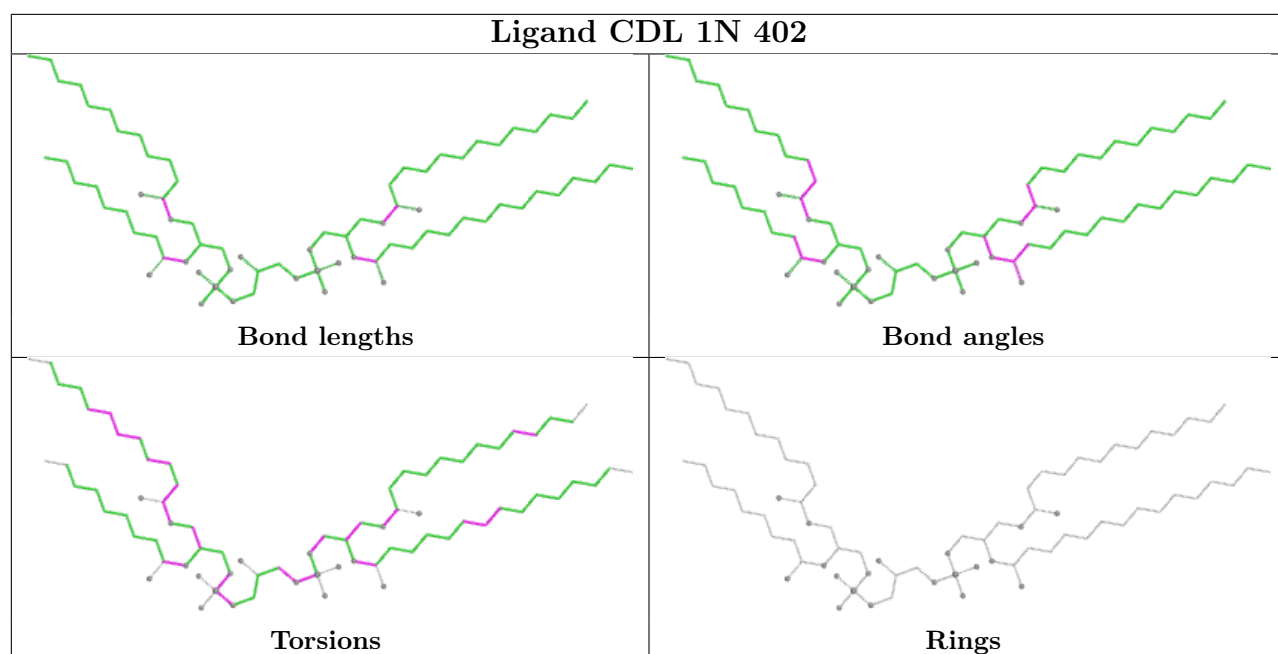


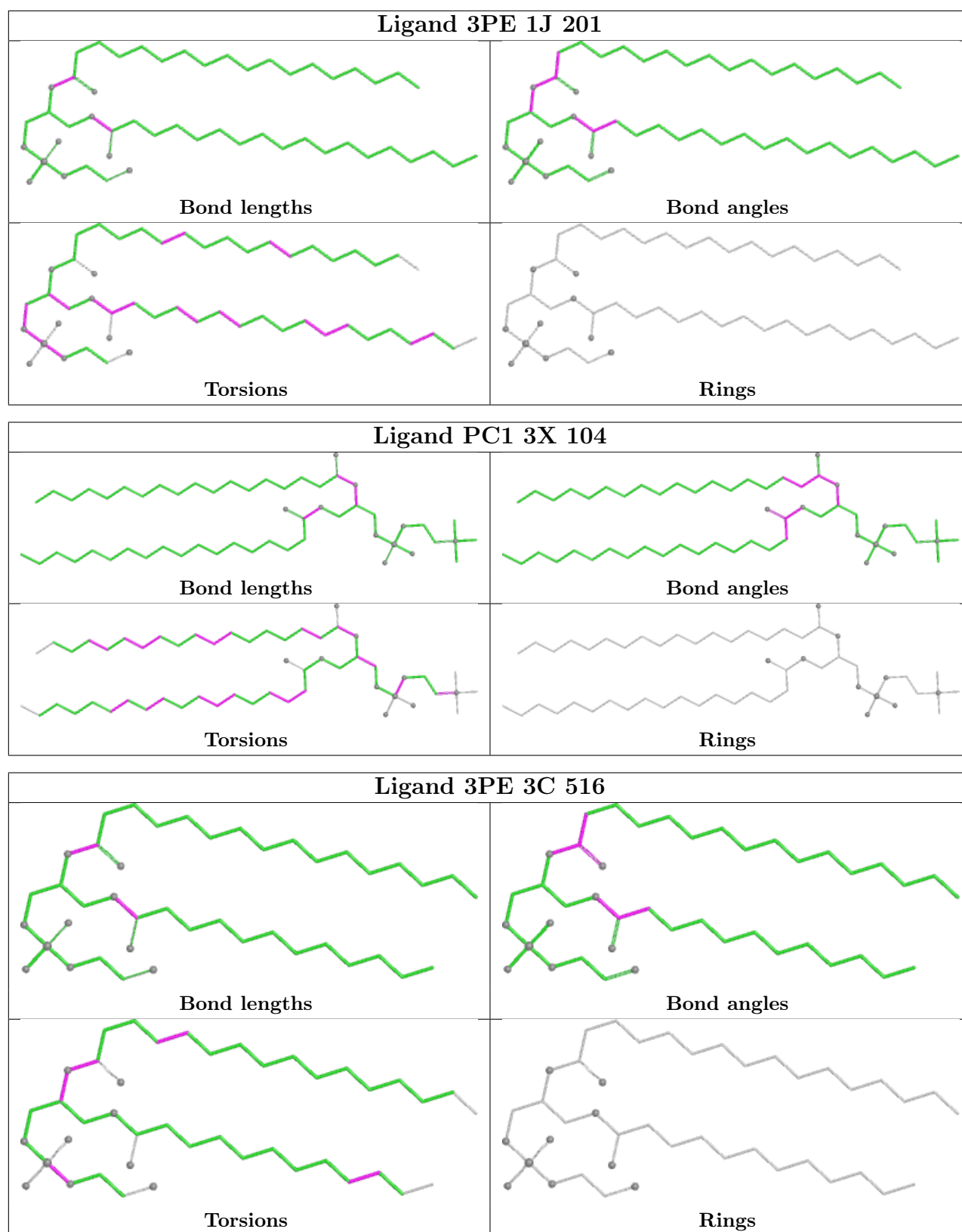












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
53	3W	3
53	3J	2
51	3G	1
52	3H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	2.65
1	3H	77:GLU	C	78:ASP	N	2.52
1	3W	57:LYS	C	58:HIS	N	2.37
1	3J	59:LYS	C	60:TYR	N	1.79
1	3J	56:ILE	C	57:LYS	N	1.07
1	3W	58:HIS	C	59:LYS	N	1.02
1	3W	56:ILE	C	57:LYS	N	0.94

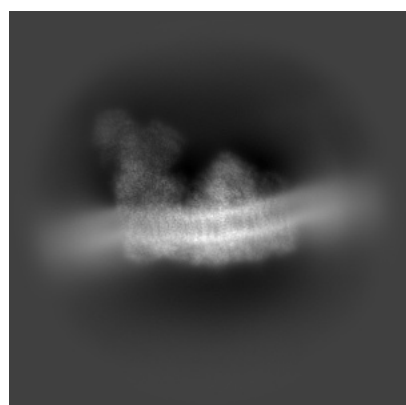
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42225. These allow visual inspection of the internal detail of the map and identification of artifacts.

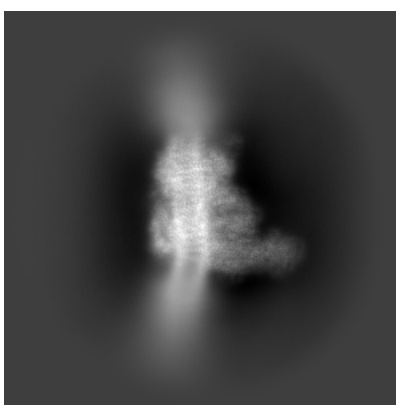
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

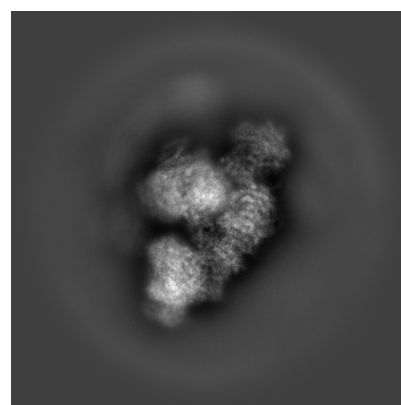
6.1.1 Primary map



X



Y

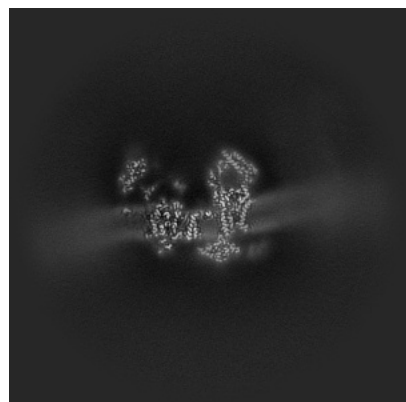


Z

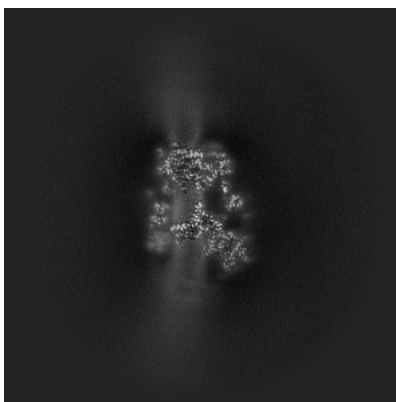
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

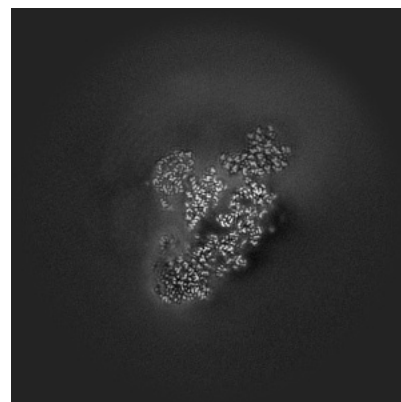
6.2.1 Primary map



X Index: 320



Y Index: 320

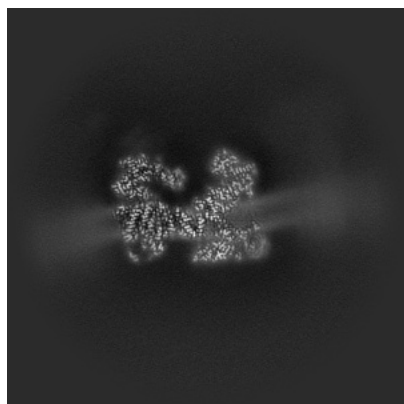


Z Index: 320

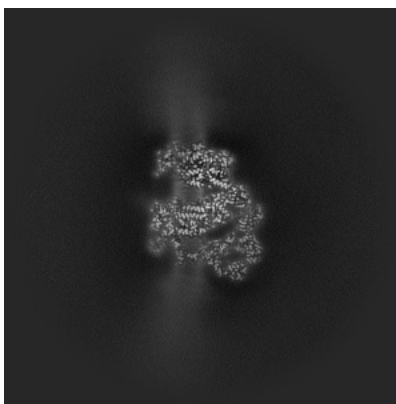
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

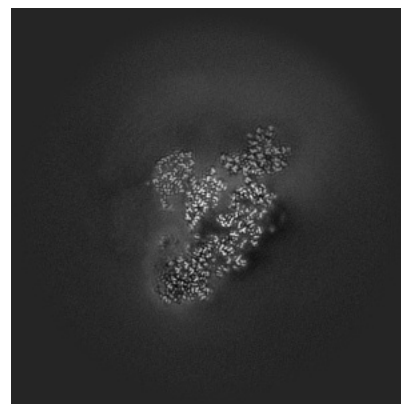
6.3.1 Primary map



X Index: 300



Y Index: 342

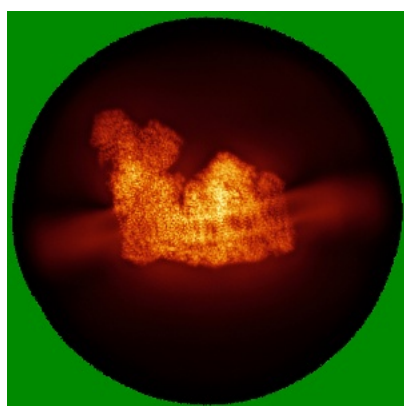


Z Index: 319

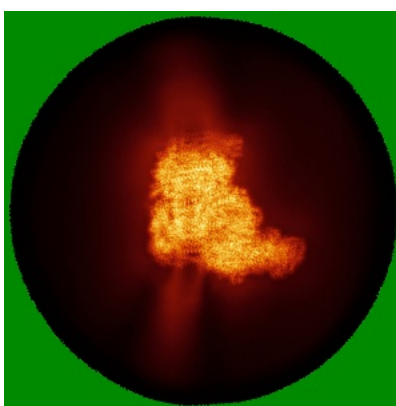
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

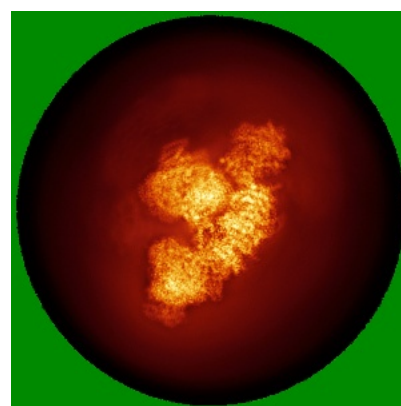
6.4.1 Primary map



X



Y

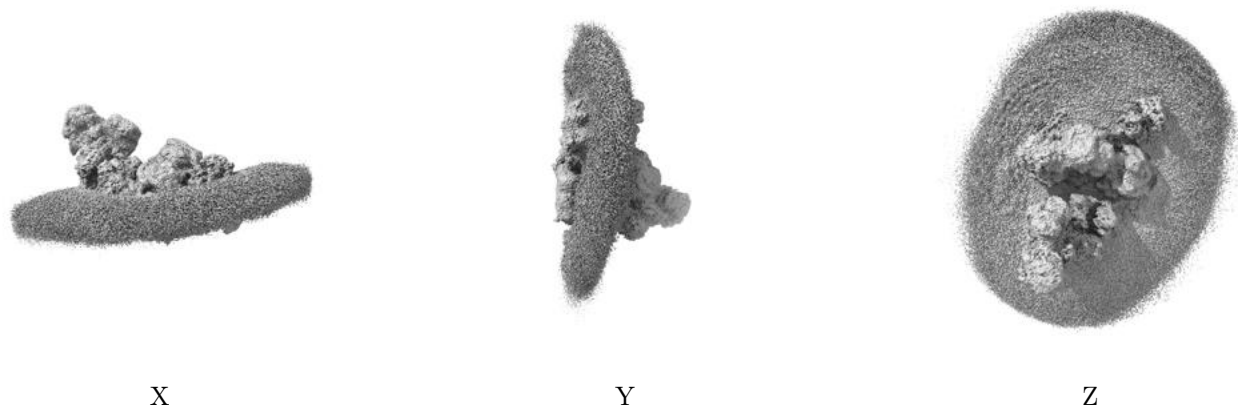


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

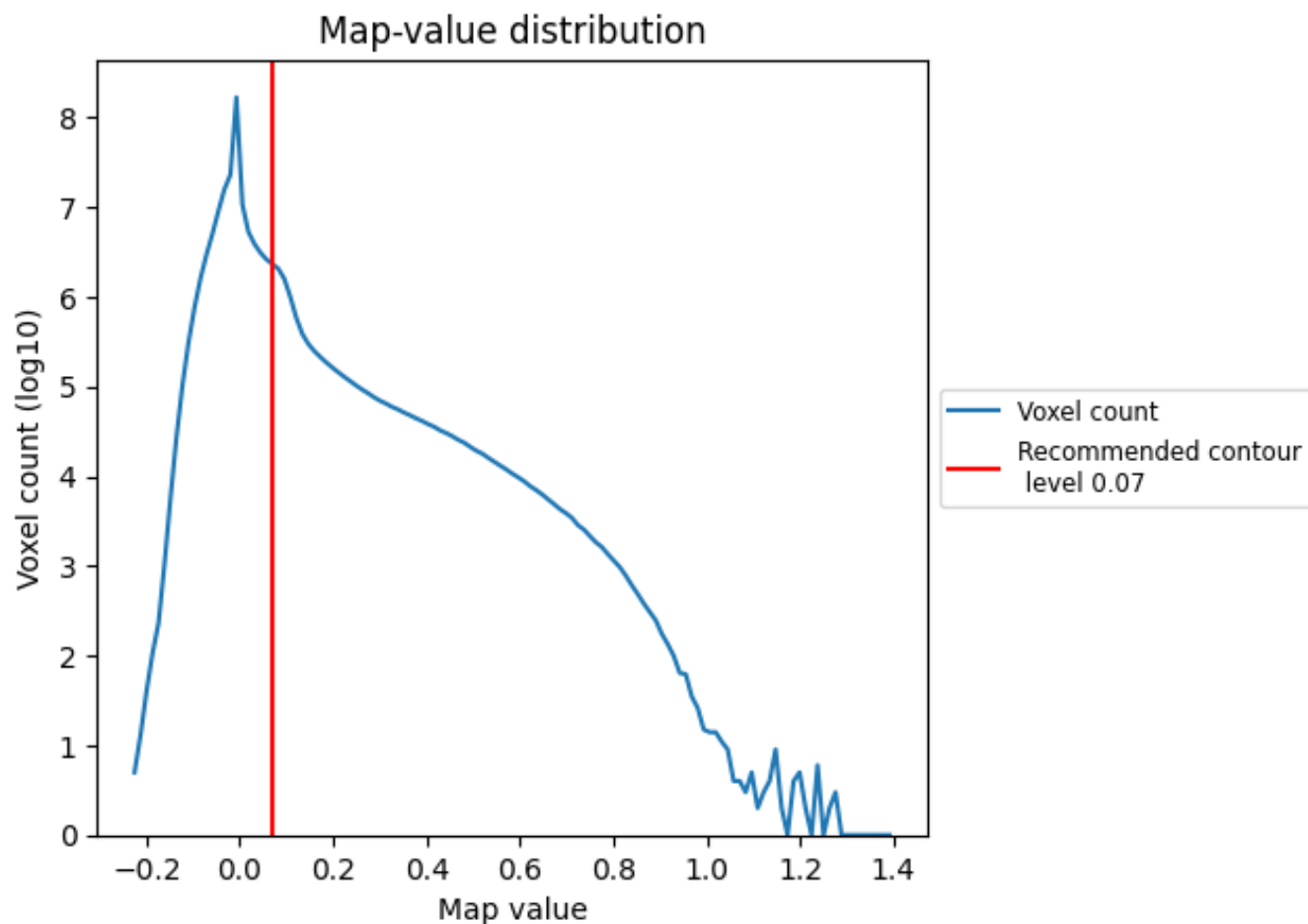
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

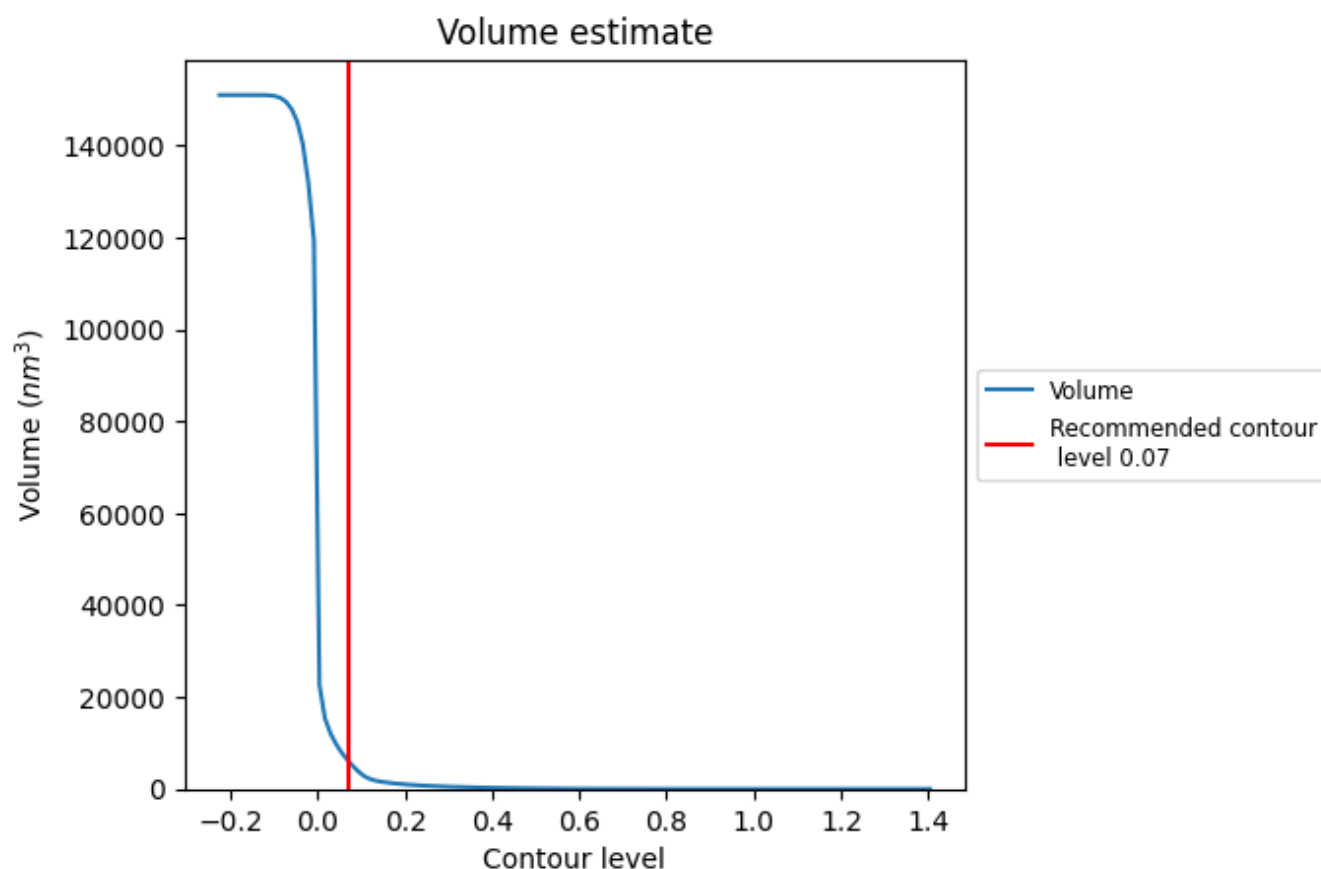
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

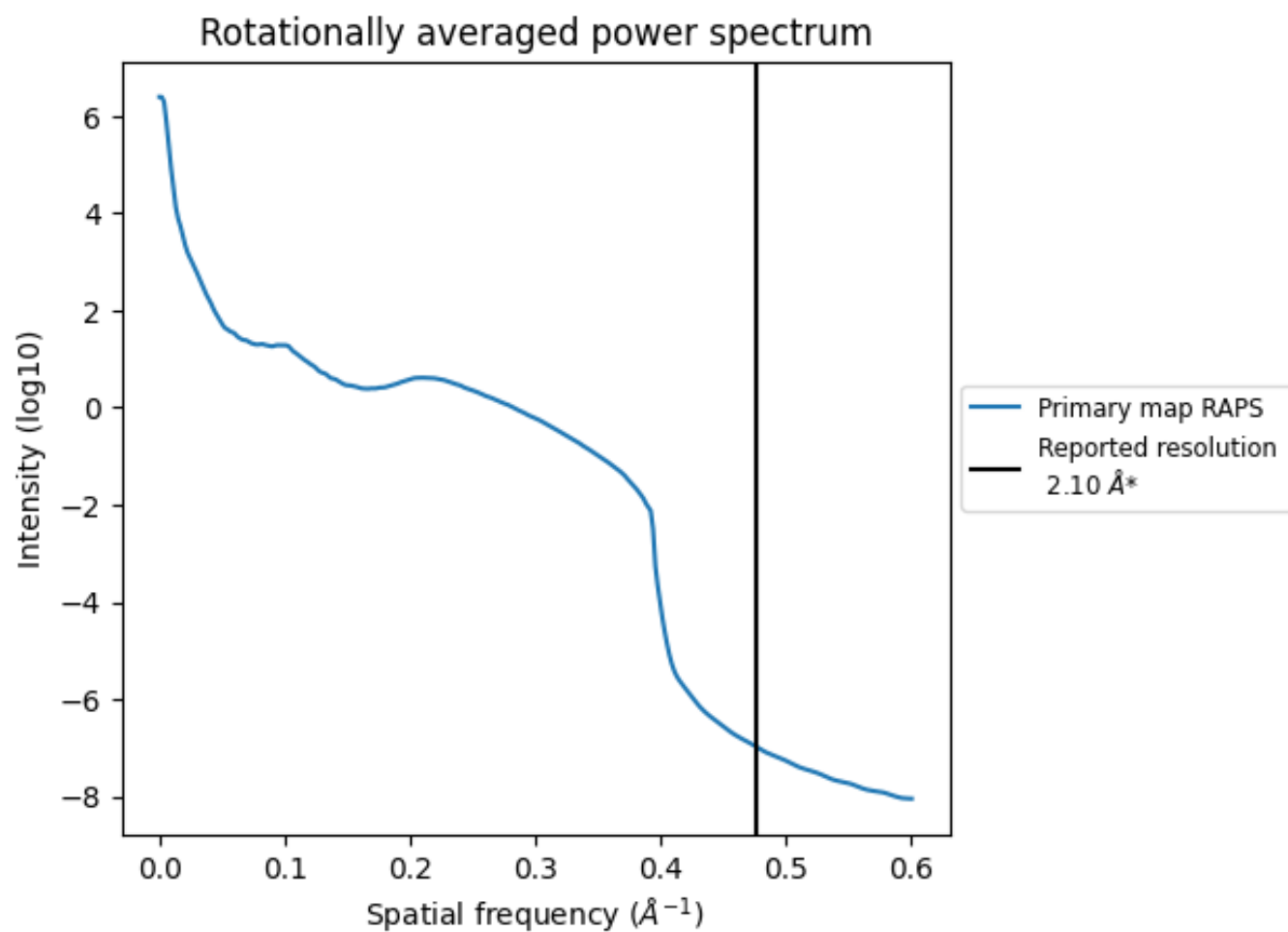
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6122 nm³; this corresponds to an approximate mass of 5530 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

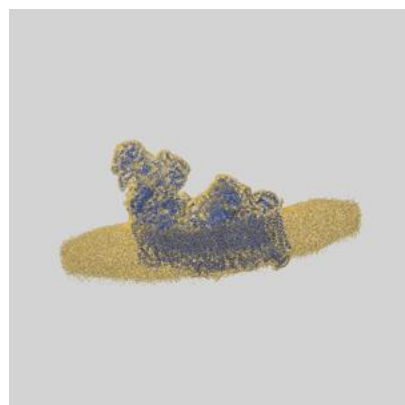
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

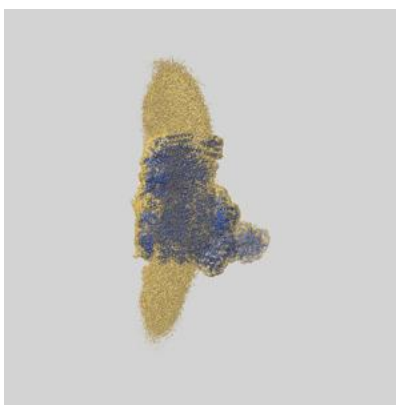
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42225 and PDB model 8UGH. Per-residue inclusion information can be found in section [3](#) on page [43](#).

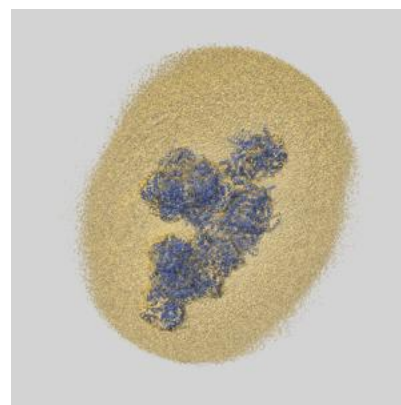
9.1 Map-model overlay [i](#)



X



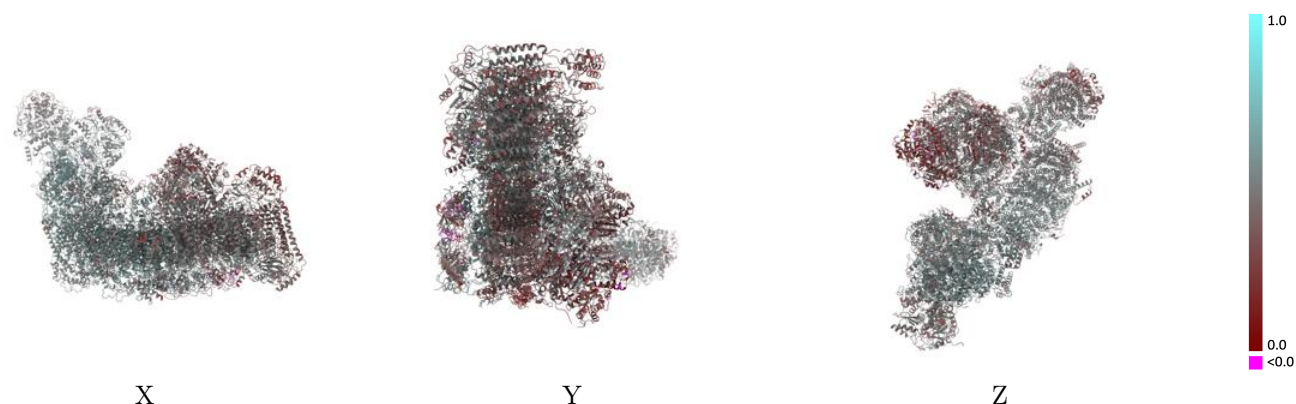
Y



Z

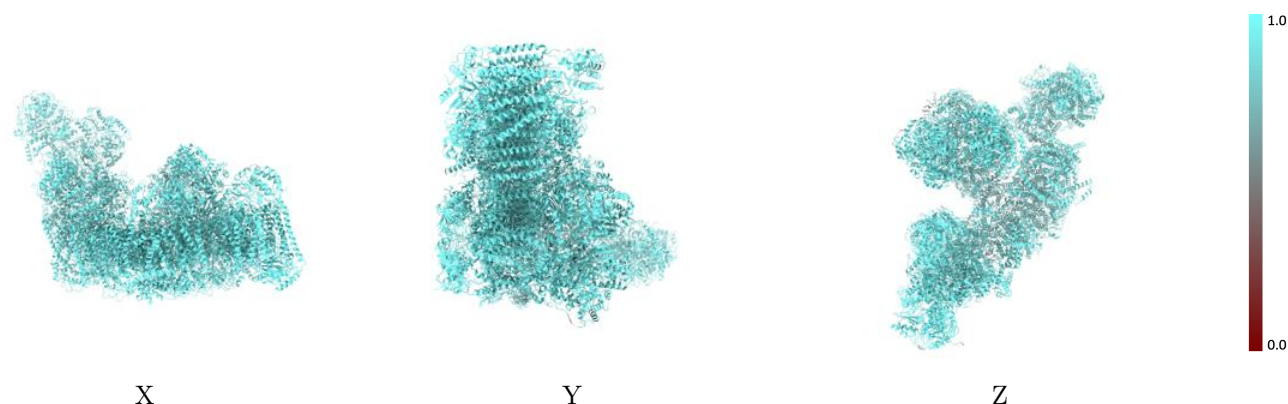
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



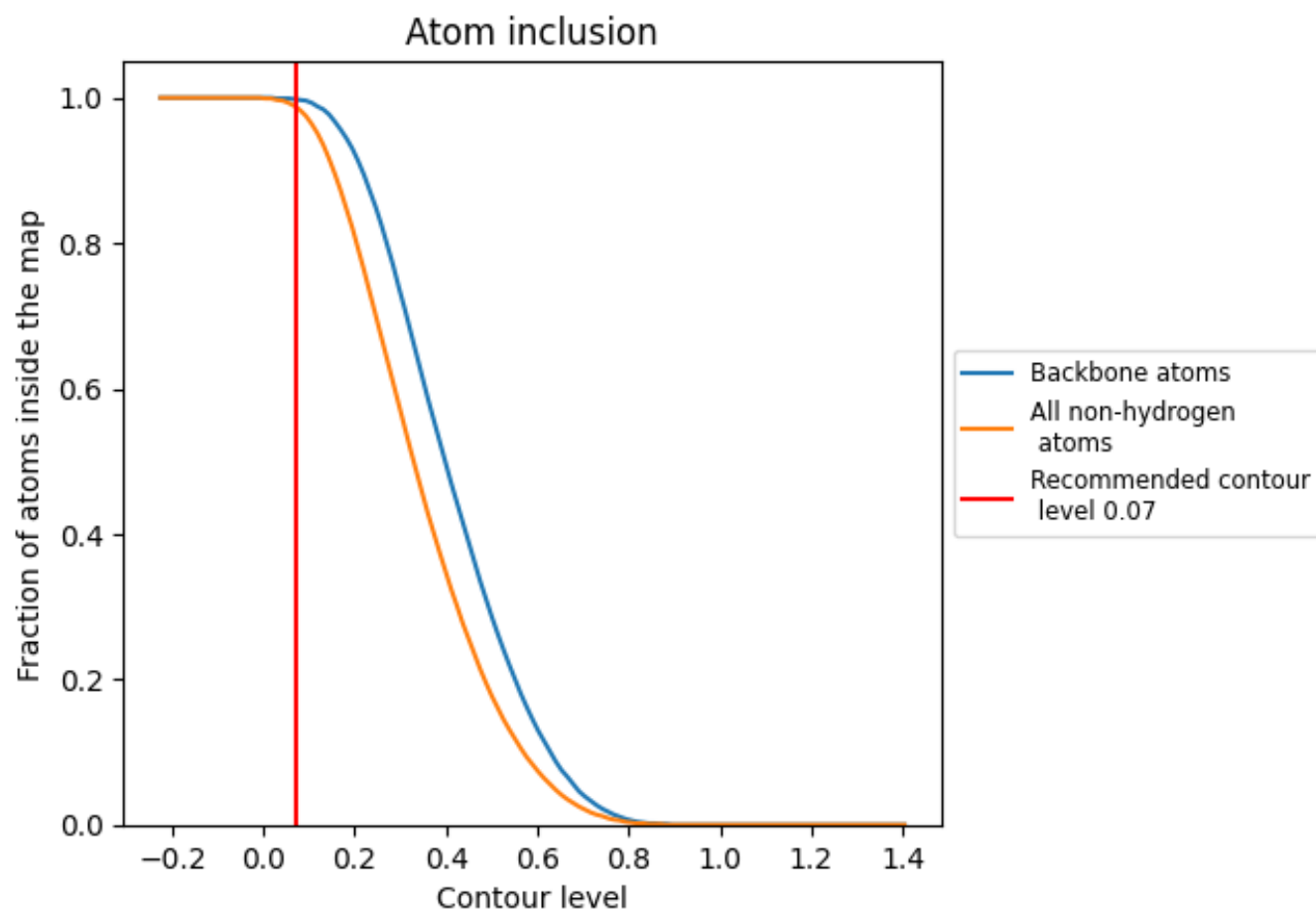
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 99% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.4640
1A	 0.9850	 0.4890
1B	 0.9970	 0.5530
1C	 0.9940	 0.5640
1D	 0.9930	 0.5690
1E	 0.9740	 0.4480
1F	 0.9800	 0.4530
1G	 0.9890	 0.4920
1H	 0.9960	 0.5470
1I	 0.9970	 0.5700
1J	 0.9970	 0.4700
1K	 0.9960	 0.5340
1L	 0.9980	 0.5100
1M	 1.0000	 0.5660
1N	 0.9990	 0.5680
1O	 0.9810	 0.5080
1P	 0.9820	 0.5060
1Q	 0.9330	 0.4950
1R	 0.9810	 0.5220
1S	 0.9720	 0.4570
1T	 0.9580	 0.3790
1U	 0.9910	 0.4370
1V	 0.9630	 0.5190
1W	 0.9640	 0.5210
1X	 0.9960	 0.5020
1Y	 0.9960	 0.4570
1Z	 0.9950	 0.5150
1a	 0.9980	 0.5440
1b	 0.9820	 0.4920
1c	 0.9850	 0.4660
1d	 0.9970	 0.5400
1e	 0.9940	 0.5000
1f	 0.9800	 0.4660
1g	 0.9920	 0.4970
1h	 0.9980	 0.5310



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Chain	Atom inclusion	Q-score
1i	 0.9930	 0.4440
1j	 0.9930	 0.4170
1k	 0.9840	 0.3990
1l	 0.9940	 0.4960
1m	 0.9990	 0.4860
1n	 0.9970	 0.4730
1o	 0.9980	 0.4490
1p	 1.0000	 0.5200
1q	 0.9960	 0.5390
1r	 0.9930	 0.5460
1s	 0.9380	 0.4160
3A	 0.9670	 0.3190
3B	 0.9820	 0.3030
3C	 0.9940	 0.4390
3D	 0.9960	 0.4890
3E	 0.9910	 0.3270
3F	 0.9540	 0.3590
3G	 0.9070	 0.3240
3H	 0.9710	 0.4230
3I	 0.9970	 0.3670
3J	 0.9960	 0.4200
3N	 1.0000	 0.4360
3O	 0.9970	 0.3550
3P	 1.0000	 0.4720
3Q	 1.0000	 0.5100
3R	 0.9890	 0.3080
3S	 1.0000	 0.4180
3T	 0.9970	 0.4580
3U	 1.0000	 0.4590
3V	 0.9910	 0.3240
3W	 1.0000	 0.4340
3X	 1.0000	 0.3610
3Y	 0.9940	 0.3390
4A	 0.9900	 0.4630
4B	 0.9900	 0.4110
4C	 0.9900	 0.4560
4D	 0.9470	 0.3920
4E	 0.9400	 0.3040
4F	 0.9290	 0.4000
4G	 0.9940	 0.4080
4H	 0.9700	 0.4090
4I	 0.9870	 0.3920

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Chain	Atom inclusion	Q-score
4J	 0.9940	 0.4810
4K	 0.9980	 0.4330
4L	 0.9650	 0.4530
4M	 0.9850	 0.4420
4N	 0.9710	 0.3780